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COMPUTER MODELING AND OPTIMIZATION
OF OBOGS WITH CONTAMINANTS

ANNUAL REPORT

JOSEPH J. BEAMAN

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19 ABSTRACT (Continue on reverse if necessary and identify by block number) / This report covers the second year of a project dealing with the development of an OBOGS computer model to aid in design and specification of these oxygen generation systems for the Army's in-flight, medivac, and field hospital use. A simple three component model using uncoupled linear isotherms has been developed but not yet tested due to a lack of data. Also, the two component model for oxygen-nitrogen has been modified to include a power law correlation for the parameters in the isotherm expressions. While this correlation is entirely empirical, it improves performance of the model at low temperatures. A major change in the project has been the transfer of the experimental duties from USAARL to UT. A preliminary set of isotherm experiments has been done (using available equipment at Brooks Air Force Base) and equipment has been ordered for the experiments to be done here at UT. The model is currently being rewritten and generalized for three components with general isotherms using a new equilibrium model.					
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STATEMENT OF PROBLEM

The ultimate goal of this research is to insure proper design of molecular sieve oxygen generation systems for the U. S. Army's in-flight, medivac, and field hospital use. Specifically the research involves further development of an OBOGS model to include the effects of contaminants in the feed air. This OBOGS model can be used to optimize and design OBOGS systems with respect to system parameters such as cycle time and bed and valve dimensions.

BACKGROUND

The pressure swing adsorption process (PSA) and its utility for oxygen generation in military applications were discussed in the last annual report (dated September 13, 1986). PSA can also be used to generate nitrogen (using zeolite 4A in the packed beds), which is useful for fuel tank inerting. See the last annual report for a discussion of the PSA process.

A major development since the last report has been the transfer of the experimental work from USAARL to UT. Thus, much effort has been expended to develop experimental techniques that will allow the determination of unknown model parameters.

APPROACH TO THE PROBLEM

Chromatographic experiments will be done to estimate model parameters. These experiments should yield information on both equilibrium and diffusion phenomena. A mass spectrometer has been ordered and should be delivered at the end of this month. This device will potentially allow for determination of ternary equilibria, where the use of isotopically labeled components may be necessary. Once the experimental arrangement has been tested against known data, work can begin on contaminants with unknown adsorptive properties. Experimental apparatus have been designed for both single column and dual column experiments.

A new equilibrium model will be implemented to allow for the use of more general isotherms in the overall model. This will eliminate the assumptions implicit in the coupling scheme presently used. The new model can predict multicomponent isotherms from pure component data. A variation of this model contains terms for "tuning" the isotherms generated if adequate experimental data exist.

In addition, the mass balance equations will probably be modified to include axial mass dispersion. Dispersion may be important at the zero velocity point in the bed.

A new computational scheme will be required to solve the new system of equations. Adaptive grid finite element methods are being considered.

RESULTS AND CONCLUSIONS

Progress has been made in two areas: experimental and computer modeling. The experimental work has just begun, while the computer work is a continuation and expansion of previous efforts.

The present computer model performs well for the oxygen-nitrogen system. This good performance is the result, to some extent, of the fact that these gases are very similar in their physical properties. The system is equilibrium dominated, so diffusional effects are minimized. Similar molecular weights and diameters further "simplify" the calculational load. Recent modifications fixed some compiler-specific "bugs" (only discovered when the model was compiled from source code at a remote location) and included a power law correlation for the isotherm parameters with temperature (see Appendix A.) (1). This temperature correlation extends the range of applicability of the model. However, these recent modifications do not address the problems that can be expected as the model is applied to more complex systems. The model is being rewritten to include multi-component feed mixtures, new equilibrium expressions and multiple mass transfer coefficients.

The number of components in the feed stream is presently fixed at two (specifically, oxygen-nitrogen). This is to be expanded to three. The properties of the third component (contaminant) are likely to differ greatly from those of oxygen and nitrogen. Therefore, simplifications possible in the oxygen-nitrogen system (such as simple isotherm forms and mass transfer expression) will not apply to the ternary system.

In the present model, oxygen is assumed to have a linear isotherm while nitrogen has a simple Langmuir-type isotherm (2). The isotherm parameters are calculated from an analysis that is specific to these isotherm forms. The isotherms are coupled using the concept of the Ideal Adsorbed Solution (3). The Ideal Adsorbed Solution Theory (IAST) is valid only for similar molecules, and is computationally intractable for ternary solutions.

As a preliminary step to a general ternary model, a limited ternary model has been developed (see Appendix B.). In its present form, this model uses uncoupled linear isotherms with a common mass transfer coefficient. The isotherm slopes are not correlated with temperature. This model represents a limiting case as the simplest possible ternary model. Unfortunately, it has not been tested due to a lack of experimental data.

The general expansion to three components presents problems in two equilibrium areas: the form of the pure component isotherm for the third component and the method of coupling the isotherms. Because the contaminant will most likely be present at low concentrations, a linear isotherm might be used. However, the contaminant will be probably be quite different from oxygen and/or nitrogen so IAST will not apply. Also, some highly polar contaminants may exhibit non-linear behavior even at low concentrations due to localized interactions in the zeolite.

A literature search has provided a model that appears to be able to solve the pure component isotherm and coupling problems. The Vacancy Solution Model (VSM) (4,5,6,7) includes terms for both adsorbate-adsorbate and adsorbate-adsorbent non-ideality. The VSM can be correlated with temperature and can include information from available binary isotherms to improve the ternary prediction. Calculation of activity coefficients may be time consuming, however, in the VSM. A sensitivity study may be done to determine if these need to be calculated at every time/distance step.

A preliminary code for the basic VSM (4,5) has been written, but not yet fully tested.

In the present model, the dynamics of mass transfer are represented in the classical form: constant mass transfer coefficient with linear driving force. The coefficient is the same for both oxygen and nitrogen; its value is determined empirically. For the oxygen-nitrogen system, performance is relatively insensitive to the value of the mass transfer coefficient because the system is equilibrium dominated (diffusion is rapid for both components). The system equations are simplified because of the common mass transfer coefficient.

Larger contaminant molecules will not diffuse as rapidly as oxygen and/or nitrogen. Therefore, at the very least, the third component will need to be considered separately. The addition of this equation may make the model stiff and more difficult to calculate. This equation will require a value for the mass transfer coefficient for the third component. At present, a literature search is underway to determine the best approach to predicting this coefficient, as well as the form of the equation. It is most likely that the present form will be retained with a separate expression for each component. However, models with the mass transfer resistance lumped at the zeolite crystal surface and bidisperse models (with resistances at both the pellet and crystal surfaces) are also being studied.

The inclusion of axial dispersion, along with the changes mentioned above, will make a new numerical scheme necessary. Finite element methods are being considered. Because

of the near "shock" phenomena expected in the concentration profiles through the beds, a very fine grid may be required for adequate resolution. Unfortunately, fine grids are very time intensive to calculate. Two adaptive grid methods are under review. One uses preset "levels" of adaptation to cause fine grids to be used where necessary; more coarse grids are used elsewhere. This method appears to suffer from the fact that nodes are being created and lost, which may complicate its implementation. The other method uses a constant number of nodes; the nodes are "moved" to form a tight grid where it is required. This method suffers from problems associated with the equations of motion for the nodes.

The main structure of the program will be changed to provide more modularity. This modularity is important in order to allow for flexibility in designing an OBOGS with the simulator. As three bed systems and systems with stratified beds (with layers of different zeolite types) become common, the model will be required to simulate them. In its present form, this will necessitate a major rewrite of the code for each change. A more modular approach will make model growth more convenient and efficient. Specifically, if temperature effects are to be addressed (i.e., a non-isothermal bed) in a future implementation of the program, it will be a great benefit if the bed equation section can be easily removed and replaced instead of rewriting the entire code.

The first structural change will be the movement of bed structure functions from the simulator program to a utility program. The designed bed systems will be stored as data files for use by the simulator. This will remove much "overhead" from the simulator as well as reduce the number of times the program needs to be recompiled when making bed parameter changes. A graphics library (for the DEC Regis VT terminals) as well as a possible structure for utility data files have been completed.

Isotherm information for many pure substances on zeolites is not readily available. Diffusion information is even more rare. Air separation data on zeolites 5A, 4A, and 13X are available in the literature because the process is important and common. However, information on other substances is either completely lacking, at inappropriate conditions (for instance, in catalytic cracking processes which operate at elevated temperatures and pressures), or "proprietary."

Therefore, experimental work must be done to determine values for necessary model parameters. Chromatographic techniques hold out the promise of obtaining both isotherm and diffusion information relatively quickly and simply (8,9). Isotherm parameters can be obtained by measuring pulse retention volumes at low flowrates. Diffusion data can be

obtained from a moments analysis on the outlet peak at higher flowrates. The moments analysis usually assumes a symmetric peak (for a pulse experiment) and linear isotherms, however; its applicability to the OBOGS problem will be unknown until some preliminary experiments have been done.

Most of the chromatographic approaches to determination of isotherm parameters usually depend on an assumption of the linear isotherm for the components at a given composition. For small enough concentration pulses, this may be a reasonable assumption. The assumption of a linear isotherm for a concentration pulse is best when an isotope of one of the components is used as the pulse (9). The pulse can then be large (because the bulk concentration will not change, no matter what the pulse size) and, consequently, more easily detected. The slope of the isotherms at each composition (which are the data obtained from the chromatographic analysis) must be integrated to obtain the isotherm itself. Then, the isotherm parameters can be estimated from the isotherm (for the VSM model (without temperature correlation) there will be three parameters to estimate). The fitting procedure used will have a critical effect on the quality of the parameters estimated. Traditional least squares analysis generally assumes all of the error is in the dependent variable. In our work, however, the independent variable (partial pressure) is also measured and subject to error. A recent paper (10) has noted that while the least squares method will fit the pure component isotherms well, the fact that the error in the independent variable was ignored will cause significant deviations when one attempts to predict binary (or higher) isotherms from these pure component parameters. Therefore, the Error-in-Variables Method (EVM) is being considered for use in parameter estimation (11). This method accounts for error in both measurements through the use of covariance matrices based on many experiments. Construction of these matrices would be quite time consuming. However, it appears as though published covariance matrices based on similar experiments may be applicable to our work (10).

Some preliminary work on the isotherm analysis has been done already, using available equipment at Brooks Air Force Base. These experiments were done in an attempt to duplicate previous work (8) in order to validate the method. Due to equipment limitations, only the binary oxygen-nitrogen isotherm was determined. Unfortunately, during the analysis of these experiments, errors were found in the mathematical derivations in (8) which led to non-physical results. The equations were solved again and physically realizable isotherms were obtained (the corrected equations are in Appendix C.). However, as the analysis in (8) was faulty, it was decided not to compare our results with those in the paper. A comparison to volumetric data on this mixture will be done (it would be better to

compare to data on the mixture at constant total pressure, but binary data of this type is rare) to check on the validity of the method.

Single and double bed apparatus have been designed for the anticipated experiments. A mass spectrometer has been ordered and is expected to arrive at the end of this month. Experimental work can then begin here at UT.

REFERENCES

1. D. Walshak, Master's Thesis, University of Texas at Austin, to be published.
2. J. J. Beaman, A. J. Healey, and J. Werlin, Trans. ASME J. Dynamic Sys., Meas., and Control, 105(1983) 265.
3. A. L. Myers and J. M. Prausnitz, AIChE J., 11(1965) 121.
4. S. Suwanayuen and R. P. Danner, AIChE J., 26(1980) 68.
5. S. Suwanayuen and R. P. Danner, AIChE J., 26(1980) 76.
6. T. W. Cochran, R. L. Kabel, and R. P. Danner, AIChE J., 31(1985) 268.
7. T. W. Cochran, R. L. Kabel, and R. P. Danner, AIChE J., 31(1985) 2075.
8. E. van der Vlist and J van der Meijden, J. Chromatography, 79(1973) 1.
9. J. J. Haydel and R. Kobayashi, Ind. Eng. Chem Fund., 6(1967) 546.
10. M. S. High and R. P. Danner, AIChE J., 32(1986) 1138.
11. P. M. Reilly and H. Patino-Leal, Technometrics, 23(1981) 221.

APPENDICES

A. Isotherm Temperature Correlation Equations

B. Simple Ternary Feed OBOGS Model

C. Corrected Equations from van der Vlist

APPENDIX A.

The temperature correlation of the isotherm parameters was entirely empirical work done by Walshak (1). Subroutines CAP1, INITIAL, and MENU need to be modified to implement the temperature correlation; they are included in this appendix. The temperature correlations are:

For oxygen:

$$K_A = .1423275 + 1.83744e-3 * (T) + 7.2443e-6 * (T)^2$$

For nitrogen:

$$K_B = .03654573 + 9.5775e-4 * (T) + 1.321e-5 * (T)^2$$

$$B = 3.059125$$

T is in degrees Celsius

```

SUBROUTINE CAP1
REAL KA,KB
COMMON/CAP/KA,KB,B,D,TEMP1
COMMON/VOID/E
KA=.1423275+.00183744*TEMP1+.0000072443*TEMP1**2
KB=.03654573+.00095775*TEMP1+.00001321*TEMP1**2
B=3.0591250818
WRITE(7,550)TEMP1,B,D,E,KA,KB
WRITE(8,550)TEMP1,B,D,E,KA,KB
550 FORMAT(' THE CURRENT BED PARAMETERS ARE:',/,
1' 12.',T5,' TEMPERATURE = ',T30,F8.3,T40,'DEGREES C',/,
2' 13.',T5,' B = ',T30,F8.4,/,
3' 14.',T5,' DIFFUSION COEFFICIENT = ',T30,F8.2,T40,'1/SEC',/,
4' 15.',T5,' VOID FRACTION = ',T30,F8.3,/,
5 T5,' AT THIS TEMPERATURE, KA = ',T30,F8.4,T40,
6 'KGMOL O2 ADSORBED/KGMOL GAS',/,
7 T5,21X,' KB = ',T30,F8.4,T40,'KGMOL N2 ADSORBED/KGMOL GAS')
RETURN
END

```

```

SUBROUTINE INITIAL(C1,C2,N1,N2,X,P)
REAL L,MA,MB,NAO1,NAO2,KA,KB,N1,N2,NBO1,NBO2,LIN
DIMENSION N1(300,2),N2(300,2),X(3),P(2)
COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,RT,AI,AO,AMWO1,AMWL1,AMWO2
1 ,AMWL2,WBR
COMMON/CAP/KA,KB,B,D,TEMP1
COMMON/VOID/E
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
C-----
C
C      RT = GAS CONSTANT*TEMP (N-M/KGMOLE)
C      AITOT,AOTOT = INLET AND OUTLET CONCENTRIC BED AREAS (M**2)
C      MA,MB = KGMOLECULAR WEIGHTS (KG/KGMOLE)
C      O,L = SUBSCRIPTS FOR Z=O AND Z=L
C      AMW = AVERAGE MOLECULAR WEIGHT (KG/KGMOLE)
C      1,2 = SUBSCRIPTS FOR BED 1 AND BED 2
C      E = VOID FRACTION
C      TEMP1 = TEMPERATURE (DEGREES C)
C-----
      RT=8314.*(TEMP1+273.16)
      AITOT=3.14159*(DIAIIN*.0254)**2/4.
      AOTOT=3.14159*(DIAOIN**2-DIAIIN**2)*.0254**2/4.
      L=.0254*LIN
      PRINT *, ' BED LENGTH (M) = ',L
      PRINT *, ' INLET BED AREA (M**2) = ',AITOT
      PRINT *, ' OUTLET BED AREA (M**2) = ',AOTOT
      MA=32.
      PRINT *, ' VOID FRACTION = ',E
      MB=28.
      AI=AITOT*E
      AO=AOTOT*E
      AMWO1=MA*X(1)+MB*(1.-X(1))
      AMWL1=MA*X(2)+MB*(1.-X(2))
      AMWO2=AMWL1
      AMWL2=MA*X(3)+MB*(1.-X(3))
      C1=P(1)*6.895E3/RT
      C2=P(2)*6.895E3/RT
      CA1=C1*X(1)
      CA2=C2*X(3)
      CB1=C1-CA1
      CB2=C2-CA2
      NBO1=(CB1/KB)/(1.+CB1/(KB*B))
      NAO1=CA1/KA
      NBO2=(CB2/KB)/(1.+CB2/(KB*B))
      NAO2=CA2/KA
      DO 1 I=1,LUMPS
      N1(I,1)=NAO1+NBO1
      N1(I,2)=NAO1
      N2(I,1)=NAO2+NBO2
1  N2(I,2)=NAO2
      DZ=L/FLOAT(LUMPS-1)
      RETURN
      END

```



```

SUBROUTINE MENU
REAL LIN,KA,KB,LIN1,KA1,KB1
DIMENSION TI(11),NY(11)
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,VO,IIN,TCYC
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,RT,AI,AO,AMWO1,AMWL1,AMWO2,
      AMWL2,WBR
COMMON/VOID/E
COMMON/CAP/KA,KB,B,D,TEMP1
COMMON/NFINISH/NEXIT
COMMON/STEP/NSTEP,TSTEP1,TSTEP2,BRSTEP
COMMON/NPRINT/NOUT1,TI,NY
NEXIT=0
NSTEP=0
10 CALL SYST1
   CALL GEOM1
   CALL CAP1
   WRITE(7,107)
   WRITE(8,107)
107 FORMAT(' ENTER CORRESPONDING PARAMETER # TO CHANGE PARAMETER',/,
1 ' ENTER "0" TO RUN SIMULATION,',
2 ' "59" TO STEP THE BREATHING FLOWRATE',/,
4 ' ENTER "99" TO EXIT PROGRAM')
N=0
READ *,N
IF(N.EQ. 0) GOTO 800
IF(N.EQ.59) GOTO 500
IF(N.EQ.99) GOTO 900
EPSI=.00000001
WRITE(7,120)
WRITE(8,120)
120 FORMAT(///,'*****',
1 //,' ENTER THE PARAMETER AND PRESS "RETURN"',/,
2//T40,'CURRENT VALUE',/)
IF(N.LT.8)GOTO 100
IF(N.LT.12)GOTO 200
IF(N.LE.18)GOTO 300
GOTO 800
100 CONTINUE
IF(N-2)159,155,155
155 IF(N-3)164,171,171
171 IF(N-4)170,175,174
159 WRITE(8,160) PSUP
WRITE(7,160) PSUP
160 FORMAT(' SUPPLY PRESSURE (PSIA)',T40,F8.4,/)
READ *,PSUP1
IF(PSUP1.LT.EPSI) GOTO 10
PSUP=PSUP1
GOTO 10
164 WRITE(8,166) POUT
166 FORMAT(' OUTLET PRESSURE (PSIA)',T40,F8.4,/)
READ *,POUT1
IF(POUT1.LT.EPSI) GOTO 10
POUT=POUT1
GOTO 10
170 WRITE(8,172) TF
172 FORMAT(' FINAL OBSERVATION TIME (SEC)',T40,F8.4,/)
READ *,TF1
IF(TF1.LT.EPSI) GOTO 10
TF=TF1
GOTO 10
175 WRITE(8,177) TCYC
177 FORMAT(' CYCLE TIME (SEC)',T40,F8.4,/)

```

```

      READ *,TCYC1
      IF(TCYC1.LT.EPSI) GOTO 10
      TCYC=TCYC1
      GOTO 10
174  WRITE(6,176) WBRL
176  FORMAT(' BREATHING MASS FLOWRATE (STD LIT/MIN) ',T40,F8.4,/)
      READ *,WBRL1
      IF(WBRL1.LT.EPSI) GOTO 178
      WBRL=WBRL1
      GOTO 10
178  GO TO 10
200  CONTINUE
      IF(N-7) 209,215,206
206  IF(N-9) 225,235,207
207  IF(N-10) 235,245,255
209  WRITE(6,210) DBYIN
210  FORMAT(' BY-PASS VALVE DIAMETER (IN) ',T40,F8.4,/)
      READ *,DBYIN1
      IF(DBYIN1.LT.EPSI) GOTO 10
      DBYIN=DBYIN1
      GO TO 10
215  WRITE(6,220) DVSIN
220  FORMAT(' SUPPLY VALVE DIAMETER (IN) ',T40,F8.4,/)
      READ *,DVSIN1
      IF(DVSIN1.LT.EPSI) GOTO 10
      DVSIN=DVSIN1
      GOTO 10
225  WRITE(6,230) DVOIN
230  FORMAT(' OUTLET VALVE DIAMETER (IN) ',T40,F8.4,/)
      READ *,DVOIN1
      IF(DVOIN1.LT.EPSI) GOTO 10
      DVOIN=DVOIN1
      GOTO 10
335  WRITE(6,240) LIN
240  FORMAT(' BED LENGTH (IN) ',T40,F8.4,/)
      READ *,LIN1
      IF(LIN1.LT.EPSI) GOTO 10
      LIN=LIN1
      GOTO 10
245  WRITE(6,250) DIAOIN
250  FORMAT(' OUTER BED DIAMETER (IN) ',T40,F8.4,/)
      READ *,DIAOIN1
      IF(DIAOIN1.LT.EPSI) GOTO 10
      DIAOIN=DIAOIN1
      GOTO 10
255  WRITE(6,260) DIAIIN
260  FORMAT(' INNER BED DIAMETER (IN) ',T40,F8.4,/)
      READ *,DIAIIN1
      IF(DIAIIN1.LT.EPSI) GOTO 10
      DIAIIN=DIAIIN1
      GOTO 10
300  CONTINUE
      IF(N-13) 309,325,305
305  IF(N-15) 335,345,10
309  WRITE(6,310) TEMP1
310  FORMAT(' TEMPERATURE (C) ',T40,F8.4,/)
      READ *,TEMP2
      IF(TEMP2.LT.EPSI) GOTO 10
      TEMP1=TEMP2
      GOTO 10
325  WRITE(6,330) B
330  FORMAT(' B ',T40,F8.4,/)
      READ *,B1

```

```

        IF(B1.LT.EPSI) GOTO 10
        B=B1
        GOTO 10
335 WRITE(6,340) D
340 FORMAT(' DIFFUSION COEFFICIENT (>100.)',T40,F8.4,/)
        READ *,D1
        IF(D1.LT.EPSI) GOTO 10
        D=D1
        GOTO 10
345 WRITE(6,350) E
350 FORMAT(' VOID FRACTION (<1.)',T40,F8.4,/)
        READ *,E1
        IF(E1.LT.EPSI) GOTO 10
        E=E1
        GOTO 10
500 WRITE(6,510) TF
        WRITE(7,510) TF
510 FORMAT(///// '-----'///,
1' ENTER THE TIME AT WHICH THE STEP CHANGE',/
2' IN BREATHING FLOWRATE IS TO OCCUR',//,
3' THE FINAL OBSERVATION TIME IS CURRENTLY ',F7.2,' SECONDS',///)
        NSTEP=1
        READ *,TSTEP1
515 WRITE(6,518) TF
        WRITE(7,518) TF
518 FORMAT(///// '-----'///,
1' ENTER THE TIME AT WHICH THE STEP CHANGE',/
2' IN BREATHING FLOWRATE IS TO END',//,
3' THE FINAL OBSERVATION TIME IS CURRENTLY ',F7.2,' SECONDS',///)
        READ *,TSTEP2
        WRITE(7,520) TSTEP1,TSTEP2,WBRL
        WRITE(6,520) TSTEP1,TSTEP2,WBRL
520 FORMAT(// '-----'///,
1' ENTER THE NEW BREATHING FLOWRATE OCCURING AS',/,
2' A STEP CHANGE FROM T= ',F7.2,' TO T= ',F7.2,' SECONDS',//,
3' THE CURRENT BREATHING FLOWRATE IS',F6.2,' STD LIT/MIN',///)
        READ *,BRSTEP
        WRITE(7,530) BRSTEP,TSTEP1,TSTEP2
        WRITE(6,530) BRSTEP,TSTEP1,TSTEP2
530 FORMAT(////,
1' -----',////,
2' THE BREATHING FLOWRATE OF ',F6.2,' STD LIT/MIN',/
3' WILL BE INPUT AS A STEP AT T= ',F7.2,' SECONDS',/
3' AND WILL END AT T= ',F7.2,' SECONDS'////,
4' -----'////)
        GOTO 10
600 CONTINUE
        WRITE(7,610)
        WRITE(6,610)
610 FORMAT(////////, '-----',////,
. ' THE FOLLOWING PLOTS ARE AVAILABLE TO YOU ON THE TERMINAL',///,
. ' 1 MOLE FRACTION OF OXYGEN VS. TIME (DATA FILE=MOLEFRAC.DAT)',/,
. ' 2 INLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)',/,
. ' 3 OUTLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)',/,
. ' 4 A DYNAMIC SIMULATION FOR ONE CYCLE (OXYGEN VS. TIME',/,
. ' DATA FILE=PROFILE.DAT)',
. //,
. ' PRESS THE CORRESPONDING # TO HAVE THE OUTPUT SHOWN AS THE',/,
. ' SIMULATION TRANSPIRES',////)
        READ(5,630)NOUT1
630 FORMAT(I1)
        IF(NOUT1.EQ.4) GOTO 750
        GO TO 400

```

```

750 DTI=1.0
DO J=1,10
TI(J)=TI(J-1)+DTI
NY(J)=IFIX(TI(J)/DT)
END DO
TI(11)=TCYC
NY(11)=IFIX(TI(11)/DT)
GO TO 400
400 WRITE(8,410)
WRITE(7,410)
410 FORMAT(////,' YOU HAVE THE FOLLOWING OPTIONS : ',
.////,T10,'1. ENTER "0" TO RUN SIMULATION.',/,
.T10,'2. ENTER "19" TO CHANGE THE PARAMETERS.',/,
.T10,'3. ENTER "99" TO EXIT PROGRAM.',////,
.' ENTER THE CORRESPONDING # AND PRESS "RETURN",////)
READ *, N69
IF(N69.EQ.0) GOTO 820
IF(N69.EQ.19) GOTO 10
IF(N69.EQ.99) GOTO 900
800 CONTINUE
WRITE(7,810)
WRITE(8,810)
810 FORMAT(////,'*****',////,
1' THE PARAMETER VALUE WAS NOT INPUT CORRECTLY',/
2' TRY AGAIN',////,'*****',////)
GOTO 10
820 WRITE(8,825)
WRITE(7,825)
825 FORMAT(////,' DO YOU WISH TO DOUBLE THE NUMBER OF SPACE LUMPS IN',/
1' THE SIMULATION FOR BETTER ACCURACY ? ( CURRENT NUMBER USED ',/
2' IS 50 ) (Y/N)',////)
READ (5,830) KEYIN
830 FORMAT ( A )
IF (KEYIN.EQ.YES) THEN
LUMPS = 101
ELSE
LUMPS = 51
END IF
GO TO 1000
900 CONTINUE
NEXIT=1
1000 RETURN
END

```

APPENDIX B.

This appendix contains the simple ternary feed OBOGS model computer code. The model uses simple linear uncoupled isotherms for all components with a common mass transfer coefficient.

```

PROGRAM MSEV
C
C OBOGS WITH CONTAMINANT
C A = COMPONENT A (OXYGEN)
C B = COMPONENT B (CONTAMINANT)
C C = COMPONENT C (NITROGEN)
C
REAL LIN,KA,KB,KC
REAL L50
BYTE CONTINUE
BYTE LOWC
BYTE KEYIN
BYTE NULL
BYTE YES
BYTE NO
CHARACTER*64 TEMP
DIMENSION W(3),XA(3),XB(3),CVA(3),PS(2),P(2)
DIMENSION WV(502,2),TV(500),XV(502,3)
DIMENSION DL(500),CA1(500),CA2(500),CB1(500),CB2(500),
1 XA1(502,11),XA2(502,11),XB1(502,11),XB2(502,11)
DIMENSION IXABS1(501,11),IYABS1(501,11),IXABS2(501,11),
1 IYABS2(501,11)
DIMENSION IX1(501),IY1(501),IX2(501),IY2(501)
DIMENSION JX(6,11),JY(6,11),JXERSH(6,11),JYERSH(6,11),
1 JXERSL(6,11),JYERSL(6,11)
DIMENSION TI(6),NY(6)
DIMENSION XCA1(502,11),XCA2(502,11),XCB1(502,11),
1 XCB2(502,11),XBR02(500)
dimension range(4),xaxis(10),yaxis(10),range2(4),xaxis2(10),
1 yaxis2(10),xaxis3(10),yaxis3(10),range3(4),
1 xaxis50(10),yaxis50(10),range50(4)
DIMENSION L50(402),T50(400),ERR(400)
COMMON/TIME/T
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,V0,IIN,TCYC
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
COMMON/CAP/KA,KB,KC,BB,BC,D
COMMON/VOID/E
COMMON/NFINISH/NEXIT
COMMON/STEP/NSTEP,TSTEP1,TSTEP2,BRSTEP
COMMON/NPRINT/NOU1,TI,NY
COMMON/BEDV/LUMPS,DZ
COMMON/HILOBED/NBED,NB
DATA CONTINUE/67/
DATA LOWC/99/
DATA NULL/0/
DATA YES/89/
DATA NO/78/
17 CALL MENU
IF ( LUMPS .EQ. 101 ) THEN
IINC = 3
ELSE
IINC = 6
END IF
IF ( NEXIT .EQ. 1 ) GOTO 900
IF ( NSTEP .EQ. 1 ) GOTO 20
TSTEP1 = 10000000.
TSTEP2 = 10000000.
BRSTEP = WBRL
20 CONTINUE
DLIN = LIN / (LUMPS-1)
DO I = 1,LUMPS
DL(I) = (I-1) * DLIN
END DO

```

```

OPEN (UNIT=1, FILE='MOLEFRAC',STATUS='NEW')
OPEN (UNIT=2, FILE='FLOWRATE',STATUS='NEW')
OPEN (UNIT=3, STATUS='SCRATCH')
OPEN (UNIT=4, FILE='PROFILE',STATUS='NEW')
OPEN (UNIT=8, STATUS='SCRATCH')
OPEN (UNIT=9, FILE='REGIS',STATUS='NEW')
OPEN (UNIT=10,FILE='CONTA',STATUS='NEW')
WRITE(6,7)
7  FORMAT(//,
1  '-----')
PRINT *
PRINT *, ' OBOGS SIMULATION'
PRINT *
IIN = 0
ND = 0
N50 = 0
CDBY = .056 / DBYIN
IF ( CDBY .GT. 1. ) CDBY = 1.
IF ( CDBY .LT. .6 ) CDBY = .6
DBYM = DBYIN * .0254
PRINT *, ' BYPASS VALVE DISCHARGE COEFFICIENT = ',CDBY
BYVA = 3.14159*DBYM**2 / 4.
VS = .8 * ( .0254*DVSIN )**2 * 3.14159 / 4.
VO = .8 * ( .0254*DVOIN )**2 * 3.14159 / 4.
PRINT *, ' AREA OF BY-PASS (M**2) = ',BYVA
PRINT *, ' CD-AREA SUPPLY VALVE (M**2) = ',VS
PRINT *, ' CD-AREA OUTLET VALVE (M**2) = ',VO
PRINT *, ' SUPPLY PRESSURE(PSI)=',PSUP,
      ' OUTLET PRESSURE(PSI)=',POUT
CVA(2) = CDBY*BYVA
T = 0.0
DT = .01
DATAP = 200.
INC = IFIX ( TF / (DATAP-DT) )
NT = 0
IM = 0
P(1) = 14.5
P(2) = 14.5
XA(2) = .20
XB(2) = 0.
PRINT *, ' BREATHING FLOW (STD LIT/MIN) = ',WBRL
XABR = .20
XBBR = 0.
IF(NOUT1-1)35,35,38
35 CLOSE(UNIT=2,STATUS='DELETE')
   CLOSE(UNIT=4,STATUS='DELETE')
   CLOSE(UNIT=9,STATUS='DELETE')
   CLOSE(UNIT=10,STATUS='DELETE')
   WRITE(1,57)
57 FORMAT(' OXYGEN MOLE FRACTION',24X,'TIME')
   GO TO 1
38 IF(NOUT1.EQ.4) GOTO 37
   IF(NOUT1.EQ.5) GOTO 170
   CLOSE(UNIT=1,STATUS='DELETE')
   CLOSE(UNIT=4,STATUS='DELETE')
   CLOSE(UNIT=9,STATUS='DELETE')
   CLOSE(UNIT=10,STATUS='DELETE')
   WRITE(2,58)
58 FORMAT(' INLET MASS FLOWRATE',T25,' OUTLET MASS FLOWRATE',
1  ' T66,TIME')
   GO TO 1
170 CLOSE(UNIT=1,STATUS='DELETE')
   CLOSE(UNIT=2,STATUS='DELETE')

```

```

CLOSE(UNIT=4,STATUS='DELETE')
CALL FRAME1
GO TO 1
37 CLOSE(UNIT=1,STATUS='DELETE')
CLOSE(UNIT=2,STATUS='DELETE')
CLOSE(UNIT=10,STATUS='DELETE')
CALL FRAME1
1 CONTINUE
XA(1) = .21
XA(3) = .21
XB(1) = .21
XB(3) = .21
CALL TIMEF ( CVA,PH,PS,T )
CALL BEDS ( P, W, XA, XB, XABR, XBRR, CVA, PS, DT,
            CA1, CA2, CB1, CB2, C1, C2 )
IF ( NOUT1 .EQ. 4 .OR. NOUT1 .EQ. 5 ) GO TO 77
GO TO 78
77 DO 1000 K=1,8
IF ( NT .EQ. NY(K) ) GO TO 150
GO TO 1000
150 CONTINUE
IF ( K .GT. 1 ) THEN

CALL INITIAL1 ( IY1(1), IY2(1), NB )
DO J=2,LUMPS
DLIN = LIN / (LUMPS-1)
DL(J) = (J-1) * DLIN
IF ( NB .EQ. 0 ) THEN
CALL DRAWF ( IX1(J), IY1(J), 1 )
ELSE
CALL DRAWF ( IX2(J), IY2(J), 1 )
END IF
END DO
CALL INITIAL2 ( IY1(1), IY2(1), NB )
DO M=2,LUMPS
IF ( NB .EQ. 0 ) THEN
CALL DRAWB ( IX2(M), IY2(M), 1 )
ELSE
CALL DRAWB ( IX1(M), IY1(M), 1 )
END IF
END DO
ELSE
END IF

DO J=2,LUMPS
DLIN = LIN / (LUMPS-1)
DL(J) = (J-1) * DLIN
END DO
IF ( TTI .GT. 0.0 ) THEN
CALL NEWTIME ( TTI,1 )
CALL NEWTIME ( TI(K),0 )
IF ( NBED .EQ. NB ) THEN
CONTINUE
ELSE
CALL FRAME2 ( NB,1 )
CALL FRAME2 ( NBED,0 )
END IF
ELSE
CALL NEWTIME ( TI(K),0 )
CALL FRAME2 ( NBED,0 )
END IF
TTI = TI(K)
IF (NOUT1 .EQ. 4) GO TO 120

```



```

      WRITE(10,-) PH,NBED,T,NT,NY(K)
      WRITE(10,110) TI(K)
      GO TO 130
120  WRITE(4,110) TI(K)
110  FORMAT('  BED COORDINATE',T20,'MOLE FRACTION IN BED#1',
1T48,'MOLE FRACTION IN BED#2',3X,'(TIME T=',F6.2,'SEC.)',/)
130  CONTINUE
      DO L=1,LUMPS
        XCA1(L,K) = CA1(L)
        XCA2(L,K) = CA2(L)
        CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        XCB1(L,K) = CB1(L)
        XCB2(L,K) = CB2(L)
        CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        IF ( NBED .EQ. 0 ) THEN
          XA1(L,K) = XCA1(L,K) / C1
          XA2(L,K) = XCA2(L,K) / C2
          CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
          XB1(L,K) = XCB1(L,K) / C1
          XB2(L,K) = XCB2(L,K) / C2
          CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
          IXABS1(L,K) = 275 + IINC*(L-1)
          IXABS2(L,K) = 575 - IINC*(L-1)
          IF ( NOUT1 .EQ. 4 ) THEN
            CALL SCALE1 ( XA1(L,K), IYABS1(L,K) )
            CALL SCALE2 ( XA2(L,K), IYABS2(L,K) )
          ELSE
            CALL SCALE1 ( XB1(L,K), IYABS1(L,K) )
            CALL SCALE2 ( XB2(L,K), IYABS2(L,K) )
          END IF
        ELSE
          M = LUMPS+1-L
          XA1(M,K) = XCA1(L,K) / C1
          XA2(M,K) = XCA2(L,K) / C2

          XB1(M,K) = XCB1(L,K) / C1
          XB2(M,K) = XCB2(L,K) / C2

          IXABS2(L,K) = 275 + IINC*(L-1)
          IXABS1(L,K) = 575 - IINC*(L-1)
          IF ( NOUT1 .EQ. 4 ) THEN
            CALL SCALE1 ( XA1(M,K), IYABS1(M,K) )
            CALL SCALE2 ( XA2(M,K), IYABS2(M,K) )
          ELSE
            CALL SCALE1 ( XB1(M,K), IYABS1(M,K) )
            CALL SCALE2 ( XB2(M,K), IYABS2(M,K) )
          END IF
        END IF
      END DO

      CALL INITIAL1 ( IYABS1(1,K), IYABS2(1,K), NBED )
      DO I=2,LUMPS
        IF ( NBED .EQ. 0 ) THEN
          CALL DRAWF ( IXABS1(I,K), IYABS1(I,K), 0 )
          IX1(I) = IXABS1(I,K)
          IY1(I) = IYABS1(I,K)
        ELSE
          CALL DRAWF ( IXABS2(I,K), IYABS2(I,K), 0 )
          IX2(I) = IXABS2(I,K)
          IY2(I) = IYABS2(I,K)
        END IF
      END DO
      DO I=1,LUMPS

```

```

      IF (NOUT1 .EQ. 4) GO TO 148
      GO TO 140
148  WRITE(4,300) DL(I), XA1(I,K), XA2(I,K)
      GO TO 180
140  WRITE(10,300) DL(I), XB1(I,K), XB2(I,K)
300  FORMAT ( 5X, F8.3, 14X, F10.6, 18X, F10.6 )
180  CONTINUE
      END DO

      CALL INITIAL2 ( IYABS1(1,K), IYABS2(1,K), NBED )
      DO 255 N=2,LUMPS
      IF ( NBED .EQ. 0 ) THEN
      CALL DRAWB ( IXABS2(N,K), IYABS2(N,K), 0 )
      IX2(N) = IXABS2(N,K)
      IY2(N) = IYABS2(N,K)
      ELSE
      CALL DRAWB ( IXABS1(N,K), IYABS1(N,K), 0 )
      IX1(N) = IXABS1(N,K)
      IY1(N) = IYABS1(N,K)
      END IF
      NB = NBED
255  CONTINUE

      XBR022 = XABR / 1.05
      DY = XBR022
      DPY = DY * 280.0
      IDY = IFIX ( DPY )
      IABS = 412 - IDY
      IF ( K .GT. 1 ) THEN
      WRITE(9,500) IA
500  FORMAT ( ' P[895,'I3']' )
      IF(IABS.LT.IA) THEN
      ID = IA - IABS
      WRITE(9,510) ID
510  FORMAT ( ' W(R,NO)V[]V[895,-'I3']' )
      ELSE
      ID = IABS - IA
      WRITE(9,520) ID
520  FORMAT ( ' W(R,N1)V[]V[895,+'I3']' )
      END IF
      ELSE
      WRITE(9,530) IABS
530  FORMAT ( ' P[895,412]V[, 'I3']' )
      END IF
      WRITE(9,535)
535  FORMAT ( ' W(NO)' )
      C      WRITE(6,200) DL(I), XA1(I,K), XA2(I,K)
      C 200 FORMAT(8X,F8.3,11X,E10.4,7X,E10.4)

      range(1) = 0.
      range(2) = 18.
      range(3) = 0.
      range(4) = 1.
      nxaxis = 20
      encode (nxaxis,258,xaxis)
258  format ( 'BED COORDINATE (IN.)' )
      nyaxis = 13
      encode (nyaxis,369,yaxis)
369  format ( 'MOLE FRACTION' )
      nxaxis50 = 11
      encode (nxaxis50,258,xaxis50)
258  format ( 'TIME (SEC.)' )
      nyaxis50 = 9

```

```

        encode (nyaxis50,366,yaxis50)
366      format ( 'L50 (IN.)' )
        IA = IABS
1000    CONTINUE
        IF (( (NOUT1.EQ.5) .AND. (MOD(NT,INC).EQ.0)) .OR. ((NOUT1.EQ.5)
        .AND. (AMOD(T,TCYC).EQ.0))) THEN
        N50 = N50 + 1
        DO M=1,LUMPS
        IF ( NBED .EQ. 0 ) THEN
        ERR(M)=(CB1(M)/C1)-.10
        ELSE
        L = LUMPS+1-M
        ERR(M) = (CB2(L)/C2) - .10
        END IF
        IF ( ABS(ERR(M)) .LE. 0.015 ) THEN
        L50(N50) = DL(M)
        ELSE
        END IF
        END DO
        T50(N50) = T
        WRITE(11,*) T50(N50),L50(N50),NBED,LUMPS
        ELSE
        END IF
        IF ( NT .EQ. NY(6) ) THEN
        RANGE50(1) = 0.
        RANGE50(2) = 0.
        RANGE50(3) = 0.
        RANGE50(4) = 0.
        CALL ZETAPLT(11,1,N50,RANGE50,T50,L50,N50+2,XAXIS50,
        NXAXIS50,,YAXIS50,NYAXIS50)
        call setaplt(10,6,lumps,range,DL,XB1,LUMPS+2,xaxis,
        nxaxis,yaxis,nyaxis)
        call setaplt(20,6,lumps,range,DL,XB2,LUMPS+2,xaxis,
        nxaxis,yaxis,nyaxis)

        CLOSE ( UNIT=9, STATUS='SAVE' )
        REWIND 9
        OPEN ( UNIT=9, FILE='REGIS', STATUS='OLD' )
        CALL TXTERASE (0)
        CALL REGISTART
        CALL PLTERASE
9200    READ ( 9, 9220, END=9999 ) TEMP
        WRITE (3,*) TEMP
        TYPE 9220,TEMP
9220    FORMAT ( A )
        GO TO 9200
9999    CALL REGISOUT
        CLOSE ( UNIT=9, STATUS='DELETE' )
        WRITE(6,9450) NULL
9450    FORMAT ( A, ' PRESS "C" TO CONTINUE : ' )
9400    READ(5,9300) KEYIN
9300    FORMAT ( A )
        IF ( KEYIN .EQ. CONTINUE .OR. KEYIN .EQ. LOWC ) THEN
        CALL TXTERASE (0)
        CALL REGISTART
        CALL PLTERASE
        CALL REGISOUT
        go to 17
        ELSE
        GO TO 9400
        END IF
        ELSE
        GO TO 8

```

```

ENDIF

78 IF ( MOD(NT,INC) ) 5,5,6
5 IM = IM + 1
  XBR02(IM) = XABR / 1.05
  IF ( NOUT1 .EQ. 1 ) THEN
    WRITE(1,84) XBR02(IM), T
84 FORMAT ( 6X, F10.6, 25X, F10.3 )
  82 IF ( ND .EQ. 0 ) THEN
    CALL TXTERASE ( 255 )
    CALL REGISTART
    CALL PLTERASE
    CALL FRAME
    TYPE 80
  80 FORMAT ( '!P[130,330]', 8 )
    GO TO 47
    ELSE
      CALL STIME ( T, IX, TF, 600., 130 )
      CALL SCALEM ( XBR02(IM), IY, 1.0, 1.0 )
      TYPE 85, IX, IY
  85 FORMAT ( '!V['I3','I3']', 8 )
    END IF
    ELSE IF ( NOUT1 .EQ. 2 ) THEN
      IF ( ND .EQ. 0 ) THEN
        CALL TXTERASE ( 255 )
        CALL REGISTART
        CALL PLTERASE
        CALL FRAME
        TYPE 86
      86 FORMAT ( '!P[130,330]', 8 )
        GO TO 47
        ELSE
          CALL STIME ( T, IX, TF, 600., 130 )
          CALL SCALEM ( WV(ND,1), IY, 0.08, 0.1 )
          TYPE 87, IX, IY
      87 FORMAT ( '!V['I3','I3']', 8 )
        WRITE(2,88) WV(ND,1), WV(ND,2), T
      88 FORMAT ( 8X, F10.6, 11X, F10.6, 10X, F10.3 )
        END IF
        ELSE IF ( NOUT1 .EQ. 3 ) THEN
          IF ( ND .EQ. 0 ) THEN
            CALL TXTERASE ( 255 )
            CALL REGISTART
            CALL PLTERASE
            CALL FRAME
            TYPE 88
          88 FORMAT ( '!P[130,330]', 8 )
            GO TO 47
            ELSE
              CALL STIME ( T, IX, TF, 600., 130 )
              CALL SCALEM ( WV(ND,2), IY, 0.08, 0.1 )
              TYPE 89, IX, IY
          89 FORMAT ( '!V['I3','I3']', 8 )
            WRITE(2,89) WV(ND,1), WV(ND,2), T
          89 FORMAT ( 8X, F10.6, 11X, F10.6, 10X, F10.6, 6X, F10.3 )
            END IF
            ELSE
              GO TO 82
            END IF
          47 CONTINUE
            ND=ND+1
            IF ( PH-180. ) 2,3,3
2 WV(ND,1)=W(3)

```

```

      WV(ND,2)=W(1)
      GO TO 4
3     WV(ND,1)=-W(1)
      WV(ND,2)=-W(3)
4     XV(ND,1)=XBR02(IM)
      XV(ND,2)=0.
      XV(ND,3)=1.
      TV(ND)=T
6     NT=NT+1
      T = NT * DT

      IF ( T .LT. TSTEP1 .AND. T .LE. TF ) THEN
        WBRLOLD = WBRL
        GO TO 1
      ELSE IF ( T .GE. TSTEP1 .AND. T .LT. TSTEP2 ) THEN
        WBRL = BRSTEP
        GO TO 1
      ELSE IF ( T .GE. TSTEP2 .AND. T .LE. TF ) THEN
        WBRL = WBRLOLD
        GO TO 1
      ELSE
        WBRL = WBRLOLD
        GO TO 18
      END IF

18    CONTINUE
      CALL REGISOUT
      WRITE(6,42) NULL
42    FORMAT ( A, ' PRESS "C" TO CONTINUE : ' )
44    READ(5,41) KEYIN
41    FORMAT ( A )
      IF ( KEYIN .EQ. CONTINUE .OR. KEYIN .EQ. LOWC ) THEN
        CALL TXTERASE (0)
        CALL REGISTART
        GO TO 43
      ELSE
        GO TO 44
      END IF
43    CALL PLTERASE
      CALL REGISOUT
      range2(1) = 0.
      range2(2) = 0.
      range2(3) = 0.
      range2(4) = 1.
      range3(1) = 0.
      range3(2) = 0.
      range3(3) = -.01
      range3(4) = .04
      nxaxis2 = 11
      encode ( nxaxis2, 257, xaxis2 )
257   format ( 'TIME (SEC.)' )
      nyaxis2 = 16
      encode ( nyaxis2, 368, yaxis2 )
368   format ( 'O2 MOLE FRACTION' )
      nxaxis3 = 11
      encode ( nxaxis3, 852, xaxis3 )
852   format ( 'TIME (SEC.)' )
      nyaxis3 = 18
      encode ( nyaxis3, 963, yaxis3 )
963   format ( 'BREATHING FLOWRATE' )
      call setaplt ( 30, 3, nd, range2, tv, xv, nd+2, xaxis2,
                     nxaxis2, yaxis2, nyaxis2 )
      call setaplt ( 40, 2, nd, range3, tv, wv, nd+2, xaxis3,

```

```

      nxaxis3, yaxis3, nyaxis3 )
100  FORMAT ( 14X, 8E12.3 )
      GO TO 17
900  WRITE(6,910)
910  FORMAT(////////'*****',////////,
1' PROGRAM TERMINATED BY OPERATOR',
2////////'*****',////////)
      END

BLOCK DATA
REAL LIN,KA,KB,KC
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,VO,IIN,TCYC
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
COMMON/CAP/KA,KB,KC,BB,BC,D
COMMON/VOID/E
DATA DT, PSUP, POUT, TF, WBRL, VS, VO, IIN, TCYC /.01,
& 40.0, 15.0, 30.0, 10.0, 0.0, 0.0, 0, 10.7 /
DATA DBYIN, DVSIN, DVOIN, LIN, DIAOIN, DIAIIN /
& .075, .306174, .43868, 15.5, 5.73, 2.18 /
DATA KA, KB, KC, BB, BC, D / .2133, .007597, .05223,
& .6414, .6265, 200. /
DATA E / .37 /
      END

SUBROUTINE MENU
REAL LIN,KA,KB,KC,LIN1,KA1,KB1,KC1
DIMENSION TI(6), NY(6), TI4(6), NY4(6), TI5(6), NY5(6)
BYTE KEYIN
BYTE YES
BYTE loyes
BYTE NO
BYTE lono
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,VO,IIN,TCYC
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,AO,AMWO1,
      AMWL1,AMWO2,AMWL2,WABR,WBBR
COMMON/VOID/E
COMMON/CAP/KA,KB,KC,BB,BC,D
COMMON/NFINISH/NEXIT
COMMON/STEP/NSTEP,TSTEP1,TSTEP2,BRSTEP
COMMON/NPRINT/NOUT1,TI,NY
DATA YES, loyes/89,121/
DATA NO, lono/78,110/
NEXIT=0
NSTEP=0
10  CALL SYST1
      CALL GEOM1
      CALL CAP1
      WRITE(7,107)
      WRITE(6,107)
107  FORMAT(' ENTER CORRESPONDING PARAMETER # TO CHANGE PARAMETER',/,
1' ENTER "0" TO SIGNIFY PARAMETERS ARE CORRECT--RUN SIMULATION',/
2' ENTER "59" TO INSERT A STEP CHANGE IN BREATHING FLOWRATE',/
4' ENTER "99" TO EXIT PROGRAM')
      N = 0
      READ *,N
      IF ( N .EQ. 0 ) GOTO 800
      IF ( N .EQ. 59 ) GOTO 500
      IF ( N .EQ. 99 ) GOTO 900
      EPSI = .0000001
      WRITE(7,120)
      WRITE(6,120)
120  FORMAT(///,'*****',

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```

1      //, ' ENTER THE PARAMETER AND PRESS "RETURN"',/,
2//T40, 'CURRENT VALUE',/)
      IF ( N .LT. 6 ) GOTO 100
      IF ( N .LT. 12 ) GOTO 200
      IF ( N .LE. 18 ) GOTO 300
      GOTO 800
100 CONTINUE
      IF ( N-2 ) 159,155,155
155 IF ( N-3 ) 164,171,171
171 IF ( N-4 ) 170,175,174
159 WRITE(6,160) PSUP
      WRITE(7,160) PSUP
160 FORMAT(' SUPPLY PRESSURE (PSIA)',T40,F8.4,/)
      READ *,PSUP1
      IF(PSUP1.LT.EPSI) GOTO 10
      PSUP=PSUP1
      GOTO 10
164 WRITE(6,166) POUT
166 FORMAT(' OUTLET PRESSURE (PSIA)',T40,F8.4,/)
      READ *,POUT1
      IF(POUT1.LT.EPSI) GOTO 10
      POUT=POUT1
      GOTO 10
170 WRITE(6,172) TF
172 FORMAT(' FINAL OBSERVATION TIME (SEC)',T40,F8.4,/)
      READ *,TF1
      IF(TF1.LT.EPSI) GOTO 10
      TF=TF1
      GOTO 10
175 WRITE(6,177) TCYC
177 FORMAT(' CYCLE TIME (SEC)',T40,F8.4,/)
      READ *,TCYC1
      IF(TCYC1.LT.EPSI) GOTO 10
      TCYC=TCYC1
      GOTO 10
174 WRITE(6,178) WBRL
178 FORMAT(' BREATHING MASS FLOWRATE (STD LIT/MIN)',T40,F8.4,/)
      READ *,WBRL1
      IF(WBRL1.LT.EPSI) GOTO 178
      WBRL=WBRL1
      GOTO 10
178 GO TO 10
200 CONTINUE
      IF(N-7) 209,215,205
205 IF(N-9) 225,235,207
207 IF(N-10) 235,245,255
209 WRITE(6,210) DBYIN
210 FORMAT(' BY-PASS VALVE DIAMETER (IN)',T40,F8.4,/)
      READ *,DBYIN1
      IF(DBYIN1.LT.EPSI) GOTO 10
      DBYIN=DBYIN1
      GO TO 10
215 WRITE(6,220) DVSIN
220 FORMAT(' SUPPLY VALVE DIAMETER (IN)',T40,F8.4,/)
      READ *,DVSIN1
      IF(DVSIN1.LT.EPSI) GOTO 10
      DVSIN=DVSIN1
      GOTO 10
225 WRITE(6,230) DVOIN
230 FORMAT(' OUTLET VALVE DIAMETER (IN)',T40,F8.4,/)
      READ *,DVOIN1
      IF(DVOIN1.LT.EPSI) GOTO 10
      DVOIN=DVOIN1

```

```

      GOTO 10
235 WRITE(6,240) LIN
240 FORMAT(' BED LENGTH (IN)',T40,F8.4,/)
      READ *,LIN1
      IF(LIN1.LT.EPSI) GOTO 10
      LIN=LIN1
      GOTO 10
245 WRITE(6,250) DIAOIN
250 FORMAT(' OUTER BED DIAMETER (IN)',T40,F8.4,/)
      READ *,DIAOIN1
      IF(DIAOIN1.LT.EPSI) GOTO 10
      DIAOIN=DIAOIN1
      GOTO 10
255 WRITE(6,260) DIAIIN
260 FORMAT(' INNER BED DIAMETER (IN)',T40,F8.4,/)
      READ *,DIAIIN1
      IF(DIAIIN1.LT.EPSI) GOTO 10
      DIAIIN=DIAIIN1
      GOTO 10
300 CONTINUE
      IF(N-13)309,315,305
305 IF(N-15)325,335,345
309 WRITE(6,310) KA
310 FORMAT ( ' KA', T40, F8.4, / )
      READ *, KA1
      IF ( KA1 .LT. EPSI ) GOTO 10
      KA = KA1
      GOTO 10
315 WRITE(6,320) KB
320 FORMAT ( ' KB', T40, F8.4, / )
      READ *, KB1
      IF ( KB1 .LT. EPSI ) GOTO 10
      KB = KB1
      GOTO 10
325 WRITE(6,330) KC
330 FORMAT ( ' KC', T40, F8.4, / )
      READ *, KC1
      IF( KC1 .LT. EPSI ) GOTO 10
      KC = KC1
      GOTO 10
335 WRITE(6,340) D
340 FORMAT(' DIFFUSION COEFFICIENT (>100.)',T40,F8.4,/)
      READ *,D1
      IF(D1.LT.EPSI) GOTO 10
      D=D1
      GOTO 10
345 WRITE(6,350) E
350 FORMAT(' VOID FRACTION (<1.)',T40,F8.4,/)
      READ *,E1
      IF(E1.LT.EPSI) GOTO 10
      E=E1
      GOTO 10
500 WRITE(6,510) TF
      WRITE(7,510) TF
510 FORMAT(/////.....'//,
1' ENTER THE TIME AT WHICH THE STEP CHANGE',/
2' IN BREATHING FLOWRATE IS TO OCCUR',//,
3' THE FINAL OBSERVATION TIME IS CURRENTLY ',F7.2,' SECONDS',///)
      NSTEP=1
      READ *,TSTEP1
515 WRITE(6,518) TF
      WRITE(7,518) TF
518 FORMAT(/////.....'//,

```



```

1' ENTER THE TIME AT WHICH THE STEP CHANGE',/
2' IN BREATHING FLOWRATE IS TO END',/,
3' THE FINAL OBSERVATION TIME IS CURRENTLY ',F7.2,' SECONDS',///)
  READ *,TSTEP2
  WRITE(7,520) TSTEP1,TSTEP2,WBRL
  WRITE(8,520) TSTEP1,TSTEP2,WBRL
520 FORMAT(//'-----',/,
1' ENTER THE NEW BREATHING FLOWRATE OCCURRING AS',/,
2' A STEP CHANGE FROM T= ',F7.2,' TO T= ',F7.2,' SECONDS',/,
3' THE CURRENT BREATHING FLOWRATE IS',F6.2,' STD LIT/MIN',///)
  READ *,BRSTEP
  WRITE(7,530) BRSTEP,TSTEP1,TSTEP2
  WRITE(8,530) BRSTEP,TSTEP1,TSTEP2
530 FORMAT(////,
1' -----',/,
2' THE BREATHING FLOWRATE OF ',F6.2,' STD LIT/MIN',/
3' WILL BE INPUT AS A STEP AT T= ',F7.2,' SECONDS',/
3' AND WILL END AT T= ',F7.2,' SECONDS'////,
4' -----'////)
  GOTO 10
800 CONTINUE
  WRITE(7,610)
  WRITE(8,610)
810 FORMAT(////////,'-----',////////,
.' THE FOLLOWING PLOTS ARE AVAILABLE TO YOU ON THE TERMINAL',/,
.' 1 MOLE FRACTION OF OXYGEN VS. TIME (DATA FILE=MOLEFRAC.DAT)',/,
.' 2 INLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)',/,
.' 3 OUTLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)',/,
.' 4 A DYNAMIC SIMULATION FOR ONE CYCLE (OXYGEN VS. TIME',/,
.' DATA FILE=PROFILE.DAT)',/,
.' 5 DYNAMIC SIMULATION OF PROPAGATION OF CONTAMINANT ALONG',/,
.' THE BED LENGTH',/,
./,/,
.' PRESS THE CORRESPONDING # TO HAVE THE OUTPUT SHOWN AS THE',/,
.' SIMULATION TRANSPIRES',////////)
  READ(5,630)NOUT1
830 FORMAT(I1)
  IF (NOUT1 .EQ. 4 ) GOTO 750
  IF (NOUT1 .EQ. 5 ) GOTO 760
  GO TO 400
750 DO J=1,5
    FJ = FLOAT(J)
    TI4(J) = 2.-FJ - 1.
    NY4(J) = IFIX ( TI4(J)/DT )
  END DO
  TI4(6) = TCYC
  NY4(6) = IFIX ( TI4(6)/DT )
  DO M=1,6
    TI(M) = TI4(M)
    NY(M) = NY4(M)
  END DO
  GO TO 400
760 DO J=2,5
    FJ = FLOAT(J)
    TI5(J) = ( TF/5. ) * (FJ-1.)
    NY5(J) = IFIX (TI5(J)/DT )
  END DO
  TI5(1) = 1.0
  NY5(1) = IFIX ( TI5(1)/DT )
  TI5(6) = TF
  NY5(6) = IFIX ( TI5(6)/DT )
  DO M=1,6
    TI(M) = TI5(M)

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```

        NY(M) = NY5(M)
        END DO
400 WRITE(6,410)
    WRITE(7,410)
410 FORMAT(////, ' YOU HAVE THE FOLLOWING OPTIONS : ',
    .////,T10,'1. ENTER "0" TO RUN SIMULATION.',/,
    .T10,'2. ENTER "19" TO CHANGE THE PARAMETERS.',/,
    .T10,'3. ENTER "99" TO EXIT PROGRAM.',////,
    . ' ENTER THE CORRESPONDING # AND PRESS "RETURN"',////)
    READ *, N89
    IF(N89.EQ.0) GOTO 820
    IF(N89.EQ.19) GOTO 10
    IF(N89.EQ.99) GOTO 900
800 CONTINUE
    WRITE(7,810)
    WRITE(6,810)
810 FORMAT(////, '-----',////,
    1' THE PARAMETER VALUE WAS NOT INPUT CORRECTLY',/
    2' TRY AGAIN',////, '-----',////)
    GOTO 10
820 WRITE(6,825)
    WRITE(7,825)
825 FORMAT(////, ' DO YOU WISH TO DOUBLE THE NUMBER OF SPACE LUMPS IN',
    1' THE SIMULATION FOR BETTER ACCURACY ? ( CURRENT NUMBER USED ',
    2' IS 50 ) (Y/N)',////)
    READ (5,830) KEYIN
830 FORMAT ( A )
    IF ( (KEYIN .EQ. YES) .OR. (KEYIN .EQ. 10yes) ) THEN
        LUMPS = 101
    ELSE
        LUMPS = 51
    END IF
    GO TO 1000
900 CONTINUE
    NEXIT = 1
1000 RETURN
    END

```

```

SUBROUTINE SYST1
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,VO,IIN,TCYC
WRITE(6,350) PSUP,POUT,TF,TCYC,WBRL
WRITE(7,350) PSUP,POUT,TF,TCYC,WBRL
350 FORMAT('    CURRENT SYSTEM PARAMETERS ARE:',/,
    1' 1. ',T5,' SUPPLY PRESSURE=',T30,F8.2,T40,'PSIA',/,
    2' 2. ',T5,' OUTLET PRESSURE=',T30,F8.2,T40,'PSIA',/,
    3' 3. ',T5,' FINAL OBSERVATION TIME=',T30,F8.2,T40,'SEC',/,
    4' 4. ',T5,' CYCLE TIME=',T30,F8.2,T40,'SEC',/,
    5' 5. ',T5,' BREATHING FLOWRATE=',T30,F8.2,T40,'STD LIT/MIN')
    RETURN
    END

```

```

SUBROUTINE GEOM1
REAL LIN
COMMON/GEOM/DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
WRITE(6,450) DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
WRITE(7,450) DBYIN,DVSIN,DVOIN,LIN,DIAOIN,DIAIIN
450 FORMAT('    CURRENT GEOMETRIC PARAMETERS ARE:',/,
    1' 6. ',T5,' BY-PASS VALVE DIAMETER = ',T30,F8.4,T40,'IN',/,
    2' 7. ',T5,' SUPPLY VALVE DIAMETER = ',T30,F8.4,T40,'IN',/,
    3' 8. ',T5,' OUTLET VALVE DIAMETER = ',T30,F8.4,T40,'IN',/,
    4' 9. ',T5,' BED LENGTH = ',T30,F8.4,T40,'IN',/,
    5' 10. ',T5,' OUTER BED DIAMETER = ',T30,F8.4,T40,'IN',/,
    6' 11. ',T5,' INNER BED DIAMETER = ',T30,F8.4,T40,'IN')

```

```

RETURN
END

```

```

SUBROUTINE CAP1
REAL KA,KB,KC
COMMON/CAP/KA,KB,KC,BB,BC,D
COMMON/VOID/E
WRITE(7,550)KA,KB,KC,D,E
WRITE(8,550)KA,KB,KC,D,E
550 FORMAT(' THE CURRENT BED PARAMETERS ARE:',/,
1' 12.',T5,' KA = ',T30,F8.4,T40,'KGMOL O2 ADSORBED/KGMOL GAS',/,
2' 13.',T5,' KB = ',T30,F8.4,T40,'KGMOL CO ADSORBED/KGMOL GAS',/,
3' 14.',T5,' KC = ',T30,F8.4,T40,'KGMOL N2 ADSORBED/KGMOL GAS',/,
4' 15.',T5,' DIFFUSION COEFFICIENT = ',T30,F8.2,T40,'1/SEC',/,
5' 16.',T5,' VOID FRACTION = ',T30,F8.3)
RETURN
END

```

```

SUBROUTINE TIMEF(CVA,PH,PS,T)
C-----CALCULATES CVA(T) AND PS(T)
DIMENSION CVA(3),PS(2)
DATA PHI,PH1,PH2,PH3,PH4,PH5,PH6/10.,20.,180.,180.,
1 200.,340.,380./
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,VO,IIN,TCYC
COMMON/HILOBED/NBED,NB
C-----
C
C PH = PHASE ANGLE OF CYCLE (DEGREES)
C TCYC = CYCLE TIME (SEC)
C
C-----
I = 0
PH = AMOD ( 360.-T/TCYC + PHI, 360. )
IF ( PH-PH1 ) 1,2,2
1 RA = PH / PH1
GO TO 11
2 IF ( PH-PH2 ) 3,4,4
3 RA = 1.
GO TO 11
4 IF ( PH-PH3 ) 5,6,6
5 RA = (PH3-PH) / (PH3-PH2)
GO TO 11
6 IF ( PH-PH4 ) 7,8,8
7 RA = (PH-PH3) / (PH4-PH3)
I = 1
GO TO 11
8 IF ( PH-PH5 ) 9,10,10
9 RA = 1.
I = 1
GO TO 11
10 RA = (PH6-PH) / (PH6-PH5)
I = 1
11 NBED = I
IF ( I ) 12,12,13
12 PS(1) = PSUP
PS(2) = POUT
CVA(1) = VS-RA
CVA(3) = VO-RA
RETURN
13 PS(1) = POUT
PS(2) = PSUP
CVA(1) = VO-RA
CVA(3) = VS-RA

```

```

RETURN
END

```

```

SUBROUTINE INITIAL (C1, C2, N1, N2, XA, XB, P )
REAL L, MA, MB, MC, NAO1, NAO2, KA, KB, KC, N1, N2, NBO1, NBO2, LIN, NCO1, NCO2
DIMENSION N1(300,3), N2(300,3), XA(3), XB(3), P(2)
COMMON/BEDV/LUMPS, DZ, L, D1, D2, MA, MB, MC, RT, AI, AO, AMWO1, AMWL1, AMWO2
1 , AMWL2, WBR
COMMON/CAP/KA, KB, KC, BB, BC, D
COMMON/VOID/E
COMMON/GEOM/DBYIN, DVSIN, DVOIN, LIN, DIAOIN, DIAIIN

```

```

C-----
C
C      RT = GAS CONSTANT*TEMP ( N-M / KGMOLE )
C      AITOT, AOTOT = INLET AND OUTLET CONCENTRIC BED AREAS ( M**2 )
C      MA, MB = KGMOLECULAR WEIGHTS ( KG / KGMOLE )
C      O, L = SUBSCRIPTS FOR Z=0 AND Z=L
C      AMW = AVERAGE MOLECULAR WEIGHT ( KG / KGMOLE )
C      1, 2 = SUBSCRIPTS FOR BED 1 AND BED 2
C      E = VOID FRACTION
C-----
C
RT = 8314. * 300.
AITOT = 3.14159 * (DIAIIN*.0254)**2 / 4.
AOTOT = 3.14159 * (DIAOIN**2-DIAIIN**2) *.0254**2 / 4.
L = .0254 * LIN
PRINT *, ' BED LENGTH (M) = ', L
PRINT *, ' INLET BED AREA (M**2) = ', AITOT
PRINT *, ' OUTLET BED AREA (M**2) = ', AOTOT
PRINT *, ' VOID FRACTION = ', E
MA = 32.
MB = 28.
MC = 28.
AI = AITOT/E
AO = AOTOT/E
AMWO1 = MA*XA(1) + MB*XB(1) + MC*(1.-XA(1)-XB(1))
AMWL1 = MA*XA(2) + MB*XB(2) + MC*(1.-XA(2)-XB(2))
AMWO2 = AMWL1
AMWL2 = MA*XA(3) + MB*XB(3) + MC*(1.-XA(3)-XB(3))
C1 = P(1)*6.895E3 / RT
C2 = P(2)*6.895E3 / RT
CA1 = C1*XA(1)
CA2 = C2*XA(3)
CB1 = C1*XB(1)
CB2 = C2*XB(3)
CC1 = C1-CA1-CB1
CC2 = C2-CA2-CB2
NAO1 = CA1 / KA
NAO2 = CA2 / KA
NBO1 = (CB1/KB) / (1.+CB1/(KB*BB))
NBO2 = (CB2/KB) / (1.+CB2/(KB*BB))
NCO1 = (CC1/KC) / (1.+CC1/(KC*BC))
NCO2 = (CC2/KC) / (1.+CC2/(KC*BC))
DO 1 I=1, LUMPS
N1(I,1) = NAO1 + NBO1 + NCO1
N1(I,2) = NAO1
N1(I,3) = NBO1
N2(I,1) = NAO2 + NBO2 + NCO2
N2(I,2) = NAO2
N2(I,3) = NBO2
1 DZ=L/FLOAT(LUMPS-1)
RETURN
END

```

```

SUBROUTINE BEDS ( P, W, XA, XB, XABR, XBBR, CVA, PS, DTG,
                  CA1, CA2, CB1, CB2, C1, C2 )
C
C-----SOLVES BED EQUATIONS
C
  REAL L,N1,N2,MA,MB,MC
  DIMENSION CA1(300),CA2(300),CB1(300),CB2(300),N1(300,3),N2(300,3),
1          G1(300,3),G2(300,3),XAT(2),XBT(2),XA0(2),XB0(2)
1          ,W(3),XA(3),XB(3),CVA(3),PS(2),PN(2),P(2)
  COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,A0,AMWO1,AMWL1,AMWO2
1          ,AMWL2,WBR
  COMMON/VOID/E
  COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,V0,IIN,TCYC
  COMMON/CAP/KA,KB,KC,BB,BC,D
  COMMON/TIME/T
C-----
C
C      C = TOTAL GAS STREAM CONCENTRATION ( KGMOLE/ M**3 )
C      CA = GAS A STREAM CONCENTRATION ( KGMOLE / M**3 )
C      N = ADSORBED PHASE CONCENTRATION ( KGMOLE / M**3 )
C      G = GAS PHASE CONCENTRATION ( KGMOLE / M**3 )
C      U = STREAM VELOCITY ( M / SEC )
C      Y = MOLECULAR FLUX ( KGMOLE / M**2-SEC )
C      L = BED LENGTH ( M )
C      D = DIFFUSION COEFFICIENT ( 1 / SEC )
C      BETA = D-AREA RATIO ( 1 / SEC )
C      DT = TIME STEP ( SEC )
C      LUMPS = NUMBER OF SPACE LUMPS
C      1,2 = SUBSCRIPTS FOR BED 1 AND BED 2
C      VBR = MIXING VOLUME FOR BREATHING FLOW ( M**3 )
C      BR = SUBSCRIPT INDICATING BREATHING VARIABLE
C      CP = PLENUM MOLE CONCENTRATION ( KGMOLE / M**3 )
C      VP = BREATHING PLENUM VOLUME ( M**3 )
C
C-----
  DT=DTG
  DO 4 I=1,2
4    PN(I) = PS(I)*6.895E3
    IF(IIN.EQ.1)GO TO 1
    IIN = 1
    CALL INITIAL ( C1, C2, N1, N2, XA, XB, P )
    VPMUL = 1.
    VP = .0018 * VPMUL
    PRINT *, ' PLENUM VOLUME (M**3) = ',VP
    DO I=1,7
    PRINT *
    END DO
    WRITE(8,10)NULL
10   FORMAT ( A, ' PLEASE WAIT.....' )
    VBR = .5*VP + .0003
    CP = .95*AMAX1( PN(1),PN(2) ) / RT
    DO 3 I=1,2
    XAT(I) = XABR
3    XBT(I) = XBBR
1    D1 = D
    D2 = D
    WBR = WBRL*4.72E-5 / 2.205
    CALL CONCEN (C1,C2,CA1,CA2,CB1,CB2,W,G1,G2,XA,XB,N1,N2,PN,CVA)
    XABR = XAT(2)
    XBBR = XBT(2)
    AMWBR = MA*XABR + MB*XBBR + MC*(1.-XABR-XBBR)
    DO 5 I=1,2
    XA0(I) = XAT(I)

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5  XBO(I) = XBT(I)
   DO 2 I=1,LUMPS
   N1(I,1) = N1(I,1) - D1*(G1(I,1)-C1)*DT
   N1(I,2) = N1(I,2) - D1*(G1(I,2)-CA1(I))*DT
   N1(I,3) = N1(I,3) - D1*(G1(I,3)-CB1(I))*DT
   N2(I,1) = N2(I,1) - D2*(G2(I,1)-C2)*DT
   N2(I,2) = N2(I,2) - D2*(G2(I,2)-CA2(I))*DT
   N2(I,3) = N2(I,3) - D2*(G2(I,3)-CB2(I))*DT
2  CONTINUE
   FAC = CP * VBR * AMWBR
   TAU1 = WBR / FAC
   XAT(1) = XA0(1) + TAU1*(XA(2)-XA0(1))*DT
   XBT(1) = XBO(1) + TAU1*(XB(2)-XBO(1))*DT
   XAT(2) = XA0(2) + TAU1*(XA0(1)-XA0(2))*DT
   XBT(2) = XBO(2) + TAU1*(XBO(1)-XBO(2))*DT
   P(1) = C1-RT / 8.895E3
   P(2) = C2-RT / 8.895E3
   AMW01 = MA*XA(1) + MB*XB(1) + MC*(1.-XA(1)-XB(1))
   AMW1 = MA*XA(2) + MB*XB(2) + MC*(1.-XA(2)-XB(2))
   AMW02 = AMW1
   AMW2 = MA*XA(3) + MB*XB(3) + MC*(1.-XA(3)-XB(3))
   RETURN
   END

   SUBROUTINE CONCEN(CG1,CG2,CA1,CA2,CB1,CB2,W,G1,G2,
1  XA,XB,N1,N2,PN,CVA)
C-----SOLVES FOR CONCENTRATIONS
   REAL L,N1,N2,MA,MB,MC
   DIMENSION CA1(300),CA2(300),CB1(300),CB2(300),N1(300,3),N2(300,3)
1  ,G1(300,3),G2(300,3)
   DIMENSION GI1(300),GI2(300),PN(2),W(3),XA(3),XB(3),CVA(3)
   COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,A0,AMW01,AMW1,AMW02
1  ,AMW2,WBR
   COMMON/VOID/E
   COMMON/VBEQ/W1,W2,W3,U01,UL1,U02,UL2,PN1,PN2,VA1,VA2,VA3
1  ,BGI1L,BGI1L2,BGI2L,BGI2L2,BL21,BL22,P1,P2
C-----
C
C   P = BED PRESSURE ( N / M**2 )
C   PN = SUPPLY PRESSURES ( N / M**2 )
C   U = STREAM VELOCITY ( M / SEC )
C   W = MASS FLOWRATE ( KG / SEC )
C   CVA = DISCHARGE COEFFICIENT TIMES VALVE AREA ( M**2 )
C   C = TOTAL GAS STREAM CONCENTRATION ( KGMOLE / M**3 )
C   CA = GAS "A" STREAM CONCENTRATION ( KGMOLE / M**3 )
C   CB = GAS "B" STREAM CONCENTRATION ( KGMOLE / M**3 )
C   CC = GAS "C" STREAM CONCENTRATION ( KGMOLE / M**3 )
C   Z = BED DISTANCE COORDINATE ( M )
C   YA = MOLECULAR FLUX OF GAS "A" = CA-U ( KGMOLE / M**2-SEC )
C   YB = MOLECULAR FLUX OF GAS "B" = CB-U ( KGMOLE / M**2-SEC )
C   XA = MOLE FRACTION OF GAS A
C   XB = MOLE FRACTION OF GAS B
C
C-----
   VA1 = CVA(1)
   VA2 = CVA(2)
   VA3 = CVA(3)
   BETA1 = (1.-E)*D1 / E
   BETA2 = (1.-E)*D2 / E
   PN1 = PN(1)
   PN2 = PN(2)
   BL21 = BETA1*.5*L
   BL22 = BETA2*.5*L

```

```

      C1 = CG1
      C2 = CG2
C-----CALCULATE G AND INTEGRAL OF G
      GI1(1) = 0.0
      GI2(1) = 0.0
      DO 1 I=1,LUMPS
        CALL CAPZ ( N1, G1, I )
1      CALL CAPZ ( N2, G2, I )
      DO 2 I=2,LUMPS
        IM1 = I-1
        GI1(I) = GI1(IM1) + DZ*( G1(I,1)+G1(IM1,1) ) / 2.
2      GI2(I) = GI2(IM1) + DZ*( G2(I,1)+G2(IM1,1) ) / 2.
      LUM2 = (LUMPS+1) / 2
      BGI1L2 = BETA1 * GI1(LUM2)
      BGI1L = BETA1*GI1(LUMPS) - BGI1L2
      BGI2L2 = BETA2 * GI2(LUM2)
      BGI2L = BETA2*GI2(LUMPS) - BGI2L2
C-----SOLVE BED/VALVE EQUATION FOR C
      CALL VAQ ( C1, C2 )
      W(1)=W1
      W(2)=W2
      W(3)=W3
      CG1=C1
      CG2=C2
C-----SOLVE FOR CONCENTRATION OF GAS A AND B
      CALL CONcab ( C1,CA1,CB1,G1,GI1,UO1,UL1,XA(1),XA(2),
1      XB(1),XB(2),BETA1,AI/AO )
      CALL CONcab ( C2,CA2,CB2,G2,GI2,UO2,UL2,XA(2),XA(3),
1      XB(2),XB(3),BETA2,AO/AI )
      RETURN
      END

      SUBROUTINE CONcab ( CG, CA, CB, G, GI, UOG, ULG, XAO, XAL,
1      XBO, XBL, BETAG, ARG )
C-----SOLVES FOR CONCENTRATION OF GAS A AND B
      REAL L2,L
      DIMENSION CA(300),CB(300),G(300,3),GI(300),XA(2),XB(2),
1      U(300),YA(300),YB(300)
      COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,AO,AMW01,AMWL1,AMW02
1      ,AMWL2,WBR
      COMMON/VOID/E
      COMMON/TIME/T
      C = CG
      BETA = BETAG
      UL = ULG
      UO = UOG
      XA(1) = XAO
      XA(2) = XAL
      XB(1) = XBO
      XB(2) = XBL
      AR = ARG
      LUM2 = (LUMPS+1) / 2
      GIL2 = GI(LUM2)
      L2 = .5*L
      IF ( UO--2 +UL--2 ) 22,22,23

C-----ZERO FLOW SOLUTION
22      DO 24 I=1,LUMPS
        CA(I) = G(I,2)
24      CB(I) = G(I,3)
      RETURN
23      CONTINUE

```

```

CA(1) = C*XA(1)
CB(1) = C*XB(1)
U(1) = UO
YA(1) = UO+CA(1)
YB(1) = UO+CB(1)
CA(LUMPS) = C*XA(2)
CB(LUMPS) = C*XB(2)
YA(LUMPS) = UL+CA(LUMPS)
YB(LUMPS) = UL+CB(LUMPS)
Z = 0.0

C-----ICR IS INDEX INDICATING U=0 IN BED

      ICR = 1
      ICR1 = ICR - 1

C-----SOLVE FOR U IN BED

      DO 3 I=2,LUMPS
      IM1 = I-1
      Z = Z+DZ
      IF ( IM1-LUM2 ) 35,34,34
35      U(I) = U(1) +BETA*( GI(I)/C - Z )
      GO TO 36
34      U(I) = AR-U(LUM2) + BETA*( (GI(I)-GIL2)/C - Z + L2 )
36      CONTINUE

C-----CHECK SIGN CHANGE OF U

      IF ( U(I)-U(IM1) ) 8,9,3
8      ICR = I
      ICR1 = ICR-1

C-----CALCULATE INTERIOR INITIAL FLUX ( UO<0, UL>0 )

      ULAST = U(IM1)
      IF ( IM1 .EQ. LUM2 ) ULAST=AR-ULAST
      DZCR = DZ*U(I) / ( U(I)-ULAST )
      DTC = DZCR - DZ
      R1 = U(ICR) / DZCR
      R3A = ( G(I,2)-G(IM1,2) ) / DZ
      R3B = ( G(I,3)-G(IM1,3) ) / DZ
      R2A = G(IM1,2) - R3A*DTC
      R2B = G(IM1,3) - R3B*DTC
      A1A = BETA+R2A+R1 / ( BETA+R1 )
      A1B = BETA+R2B+R1 / ( BETA+R1 )
      A2A = BETA+R3A+R1 / ( BETA+2.-R1 )
      A2B = BETA+R3B+R1 / ( BETA+2.-R1 )
      YA(ICR) = A1A-DZCR + A2A-DZCR-DZCR
      YB(ICR) = A1B-DZCR + A2B-DZCR-DZCR
      YA(ICR1) = A1A-DTC + A2A-DTC-DTC
      YB(ICR1) = A1B-DTC + A2B-DTC-DTC
      CA(ICR) = YA(ICR) / U(ICR)
      CB(ICR) = YB(ICR) / U(ICR)
      CA(ICR1) = YA(ICR1) / ULAST
      CB(ICR1) = YB(ICR1) / ULAST
      GO TO 3
9      ICR = I
      ICR1 = I
      YA(ICR) = 0.0
      YB(ICR) = 0.0
      IF ( UO ) 3,25,3
25      ICR = 1

```



```

      ICR1 = 1
      YA(1) = 0.0
      YB(1) = 0.0
3      CONTINUE
      UL = U(LUMPS)
C-----LOGIC FOR FORWARD INTEGRATION
      ISIG = 1
      IF ( UL ) 14,14,15
14     IST = 1
      IF ( UO ) 12,20,21
21     CONTINUE
      IT = ICR-2
      IF ( IT ) 12,12,11
20     ICR = 1
      ICR1 = 1
      GO TO 12
15     CONTINUE
      IST = ICR
      IT = LUMPS-ICR
      IF ( IT ) 12,12,11
11     CONTINUE

C-----SOLVE FOR CA

      DO 10 J=1,IT
      I = IST + ISIG*J
      IM1 = I-ISIG
      IF ( IM1-LUM2 ) 33,30,33
30     IF ( ISIG ) 31,33,32
31     YA(IM1) = YA(IM1) / AR
      YB(IM1) = YB(IM1) / AR
      U(IM1) = U(IM1) / AR
      GO TO 33
32     U(IM1) = AR*U(IM1)
      YA(IM1) = AR*YA(IM1)
      YB(IM1) = AR*YB(IM1)
33     CONTINUE
      RO = U(IM1)
      IF ( I .EQ. LUM2 .AND. ISIG .EQ. -1 ) U(I)=AR*U(I)
      R1 = ( U(I)-RO ) / DZ
      R2A = G(IM1,2)
      R2B = G(IM1,3)
      R3A = ( G(I,2)-R2A ) / DZ
      R3B = ( G(I,3)-R2B ) / DZ
      IF ( R1 ) 8,7,6
7      AOA = ( R2A-R3A*RO/BETA ) * RO
      AOB = ( R2B-R3B*RO/BETA ) * RO
      A1A = R3A*RO
      A1B = R3B*RO
      BR = BETA / RO
      YA(I) = ( YA(IM1)-AOA )*EXP(-BR*DZ) + AOA + A1A*DZ
      YB(I) = ( YB(IM1)-AOB )*EXP(-BR*DZ) + AOB + A1B*DZ
      GO TO 10
8      A2A = BETA*R3A*R1 / ( BETA+2.*R1 )
      A2B = BETA*R3B*R1 / ( BETA+2.*R1 )
      A1A = ( BETA*(R3A*RO+R2A*R1) - 2.*A2A*RO ) / ( BETA+R1 )
      A1B = ( BETA*(R3B*RO+R2B*R1) - 2.*A2B*RO ) / ( BETA+R1 )
      AOA = ( BETA*RO-R2A-A1A*RO ) / BETA
      AOB = ( BETA*RO-R2B-A1B*RO ) / BETA
      IF ( RO ) 28,27,26
27     YA(I) = A1A*DZ + A2A*DZ*DZ
      YB(I) = A1B*DZ + A2B*DZ*DZ
      GO TO 28

```

```

26  CONTINUE
    BR = BETA/R1
    YA(I) = ( YA(IM1)-AOA )*( 1.+R1-DZ/RO )*(-BR) + AOA + A1A-DZ
           + A2A-DZ-DZ
    YB(I) = ( YB(IM1)-AOB )*( 1.+R1-DZ/RO )*(-BR) + AOB + A1B-DZ
           + A2B-DZ-DZ
28  CONTINUE
    IF ( U(I) ) 18,19,18
19  CA(I) = C-G(I,2) / G(I,1)
    CB(I) = C-G(I,3) / G(I,1)
    GO TO 10
18  CA(I) = YA(I) / U(I)
    CB(I) = YB(I) / U(I)
10  CONTINUE
    IF ( ICR .EQ. 1 ) GO TO 13
    IF ( DZ ) 13,13,12
12  CONTINUE

```

C-----LOGIC FOR BACKWARD INTEGRATION

```

    DZ = -DZ
    ISIG = -1
    IF ( UL ) 16,16,17
16  IST = LUMPS
    IT = LUMPS - ICR
    IF ( ICR .EQ. ICR1 ) IT=IT-1
    IF ( IT ) 13,13,11
17  CONTINUE
    IST = ICR1
    IT = ICR1-1
    IF ( IT ) 13,13,11
13  CONTINUE
    XA(1) = CA(1) / C
    XA(2) = CA(LUMPS) / C
    XB(1) = CB(1) / C
    XB(2) = CB(LUMPS) / C
    DZ = FLOAT(ISIG) * DZ
    XAO = XA(1)
    XAL = XA(2)
    XBO = XB(1)
    XBL = XB(2)
    RETURN
END
SUBROUTINE CAPZ ( N, G, I )
REAL KA,KB,KC,N,NA,NB,NC
DIMENSION N(300,3),G(300,3)
COMMON/CAP/KA,KB,KC,BB,BC,D
NA = N(I,2)
NB = N(I,3)
NC = N(I,1) - NA - NB
G(I,2) = KA-NA
G(I,3) = KB-NB / (1.-NB/BB )
GC = KC-NC / (1.-NC/BC )
G(I,1) = G(I,2) + G(I,3) + GC
RETURN
END
SUBROUTINE VALVE ( A, PU, PD, W )

```

C-----CALCULATES VALVE MASS FLOWRATE KG/SEC

```

REAL KI
DATA KI, C1, C2, CK / .714, .00906, .00234, .286 /
PUL = PU
PDL = PD
PR = PDL / PUL

```

```

      SIG = 1.
      IF ( 1.-PR ) 4,3,2
3     W = 0.
      RETURN
4     PR = 1. / PR
      PUL = PDL
      SIG = -1.
2     CONTINUE
      IF ( PR .LT. .528 ) GO TO 1
      PRR = 1. - PR--CK
      W = SIG-A-C1-PUL-(PR--KI)-SQRT(PRR)
      RETURN
1     W = SIG-A-C2-PUL
      RETURN
      END
      SUBROUTINE VAQ ( CG1, CG2 )
C-----ITERATION AND FALSE POSITION TO SOLVE VALVE/BED EQUATIONS
      EXTERNAL F1,F2
      COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,AO,AMWO1,AMWL1,AMWO2
1     ,AMWL2,WBR
      COMMON/VBEQ/W1,W2,W3,UO1,UL1,UO2,UL2,PN1,PN2,VA1,VA2,VA3
1     ,BGI1L,BGI1L2,BGI2L,BGI2L2,BL21,BL22,P1,P2
      C1 = CG1
      C2 = CG2
      P1 = C1-RT
      P01 = P1
      J = 1
10    FC2 = F2 ( C2 )
1     CN2 = C2-( 1.-FC2 )
      IF ( ABS(CN2-C2)/C2 .LE. 1.E-6 ) GO TO 2
      FCN2 = F2 ( CN2 )
      IF ( FC2-FCN2 ) 4,3,3
3     C2 = CN2
      FC2 = FCN2
      GO TO 1
4     C2 = FP ( F2, FCN2, CN2, FC2, C2 )
2     CONTINUE
      FC1 = F1 ( C1 )
5     CN1 = C1-( 1.-FC1 )
      IF ( ABS(CN1-C1)/C1 .LE. 1.E-6 ) GO TO 6
      FCN1 = F1 ( CN1 )
      IF ( FC1-FCN1 ) 8,7,7
7     C1 = CN1
      FC1 = FCN1
      GO TO 5
8     C1 = FP ( F1, FCN1, CN1, FC1, C1 )
6     IF ( ABS(P1-P01)/P1 .LE. 1.E-6 ) GO TO 9
      J = J+1
      P01 = P1
      IF ( J .LE. 20 ) GO TO 10
      PRINT 100
100   FORMAT ( 1X, '-FAILED TO CONVERGE-' )
9     CG1 = C1
      CG2 = C2
      RETURN
      END
      FUNCTION F1 ( CG1 )
C-----BED 1 VALVE/BED EQUATION
      COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,AO,AMWO1,AMWL1,AMWO2
1     ,AMWL2,WBR
      COMMON/VBEQ/W1,W2,W3,UO1,UL1,UO2,UL2,PN1,PN2,VA1,VA2,VA3
1     ,BGI1L,BGI1L2,BGI2L,BGI2L2,BL21,BL22,P1,P2
      C1 = CG1

```

```

P1 = C1*RT
CALL VALVE ( VA1, PN1, P1, W1 )
CALL VALVE ( VA2, P1, P2, W2 )
IF ( P1-P2 ) 1,2,3
1  WBR1 = 0.
   GO TO 4
2  WBR1 = .5-WBR
   GO TO 4
3  WBR1 = WBR
4  CONTINUE
   UO1 = W1 / ( C1-AMWO1*AI )
   UL1 = ( W2+WBR1 ) / ( C1-AMWL1*AO )
   AR = AI / AO
   F1 = 1. - ( AR*BGI1L2+BGI1L ) / ( (UL1+BL21-AR*(UO1-BL21))*C1 )
   RETURN
   END
FUNCTION F2 ( CG2 )
C-----BED 2 VALVE/BED EQUATION
COMMON/BEDV/LUMPS,DZ,L,D1,D2,MA,MB,MC,RT,AI,AO,AMWO1,AMWL1,AMWO2
1 ,AMWL2,WBR
COMMON/VBEQ/W1,W2,W3,UO1,UL1,UO2,UL2,PN1,PN2,VA1,VA2,VA3
1 ,BGI1L,BGI1L2,BGI2L,BGI2L2,BL21,BL22,P1,P2
   C2 = CG2
   P2 = C2*RT
   CALL VALVE ( VA2, P1, P2, W2 )
   CALL VALVE ( VA3, P2, PN2, W3 )
   IF ( P2-P1 ) 1,2,3
1  WBR2 = 0.
   GO TO 4
2  WBR2 = .5-WBR
   GO TO 4
3  WBR2 = WBR
4  CONTINUE
   UO2 = ( W2-WBR2 ) / ( C2-AMWO2*AO )
   UL2 = W3 / ( C2-AMWL2*AI )
   AR = AO / AI
   F2 = 1. - ( AR*BGI2L2+BGI2L ) / ( (UL2+BL22-AR*(UO2-BL22))*C2 )
   RETURN
   END
FUNCTION FP ( F, FXR, XR, FXL, XL )
C-----USES FALSE POSITION TO FIND ZERO
DATA EPS / 1.E-6 /
   I = 0
3  X = XL -FXL*(XL-XR) / ( FXL-FXR )
   FX = F ( X )
   I = I+1
   IF ( ABS(FX) .LT. EPS ) GOTO 4
   IF ( I .GT. 50 ) GOTO 4
   IF ( FX*FXL ) 1,1,2
1  XR = X
   FXL = FXL-FXR / ( FXR+FX )
   FXR = FX
   GOTO 3
2  XL = X
   FXR = FXR-FXL / ( FXL+FX )
   FXL = FX
   GOTO 3
4  FP = X
   RETURN
   END

```

```

subroutine zetaplt(nplot,ncvs,npts,range,x,y,ny,xaxis,hxaxis,
yaxis,nyaxis)

```

```

dimension x(300),y(302,11),c(6),range(4),xaxis(10),yaxis(10)
data axlenx,axleny / 7.0, 5.0 /
call plots ( 0, 0, nplot )
call plot ( 0.5, 0.5, -3 )
call factor ( 0.65 )
if ( (range(1).eq.0.) .and. (range(2).eq.0.) ) then
  call scale ( x, axlenx, npts, 1 )
else
  x(npts+1) = range(1)
  x(npts+2) = (range(2)-range(1))/axlenx
end if
if ( (range(3).eq.0.) .and. (range(4).eq.0.) ) then
  call scale ( y, axleny, npts, 1 )
else
  y(npts+1,1) = range(3)
  y(npts+2,1) = (range(4)-range(3))/axleny
end if
if ( ncvs .ge. 2 ) then
  do n = 2,ncvs
    y(npts+1,n) = y(npts+1,1)
    y(npts+2,n) = y(npts+2,1)
  end do
end if
call axis ( 0.0, 0.0, xaxis, -nxaxis, axlenx, 0.0,
           x(npts+1), x(npts+2) )
call axis ( 0.0, 0.0, yaxis, nyaxis, axleny, 90.0,
           y(npts+1,1), y(npts+2,1) )
do m = 1,ncvs
  call line ( x, y(1,m), npts, 1, 0, 2 )
end do
call plot ( 0.0, 0.0, 999 )
return
end

SUBROUTINE SCALE1 ( Y, YABS )
COMMON/HILOBED/NBED
INTEGER YABS
DY = 1.0 - Y
DPY = DY * 150.0
IDY = IFIX ( DPY )
YABS = IDY + 100
RETURN
END

SUBROUTINE SCALE2 ( Y, YABS )
COMMON/HILOBED/NBED
INTEGER YABS
DY = 1.0 - Y
DPY = DY * 150.0
IDY = IFIX ( DPY )
YABS = IDY + 300
RETURN
END

SUBROUTINE INITIAL1 ( YABS1, YABS2, NBED )
INTEGER YABS1,YABS2
IF ( NBED .EQ. 0 ) THEN
  WRITE(9,100) YABS1
ELSE
  WRITE(9,100) YABS2
END IF
END IF
100 FORMAT (3X, ' P[275,'I3']' )
RETURN
END

SUBROUTINE INITIAL2 ( YABS1, YABS2, NBED )

```

```

        INTEGER YABS1,YABS2
        IF ( NBED .EQ. 0 ) THEN
            WRITE(9,100) YABS2
        ELSE
            WRITE(9,100) YABS1
        END IF
100  FORMAT (3X, ' P[575,'I3']' )
        RETURN
    END
    SUBROUTINE DRAWF ( XABS, YABS, NM )
C DRAW VECTORS FROM PREVIOUS CURSOR POSITIONS TO CURRENT POINTS
C FORWARD PLOTTING
    INTEGER XABS, YABS
    WRITE(9,100) NM,XABS,YABS
100  FORMAT (3X, ' W(R,N'I1')V[]V['I3','I3']' )
    RETURN
    END
    SUBROUTINE DRAWB ( XABS, YABS, NM )
C BACKWARD PLOTTING
    INTEGER XABS,YABS
    WRITE(9,100) NM, XABS, YABS
100  FORMAT (3X, ' W(R,N'I1')V[]V['I3','I3']' )
    RETURN
    END
    SUBROUTINE TXTERASE (NTICKS)
C ERASE THE VT125 TEXT SCREEN
    LOGICAL ERASE
    DIMENSION ERASE(4)
    DATA ERASE / 27, '[', '2', 'J' /
    IF ( NTICKS.NE.0 ) THEN
        DO I=1,7
            CALL DELAY (NTICKS)
        END DO
    ELSE
        END IF
    TYPE 10, ERASE
10  FORMAT ( '+', 5A1, 8 )
    RETURN
    END
    SUBROUTINE REGISTART
C SETS VT125 INTO GRAPHICS(REGIS) MODE
    LOGICAL GRAPHIC
    DIMENSION GRAPHIC(3)
    DATA GRAPHIC / 27, 'P', 'p' /
    TYPE 10, GRAPHIC
10  FORMAT ( '+', 5A1, 8 )
    RETURN
    END
    SUBROUTINE PLTERASE
C ERASES PLOTS
    LOGICAL ERASE
    DIMENSION ERASE(4)
    DATA ERASE / 'S', '(', 'E', ')' /
    TYPE 10, ERASE
10  FORMAT ( '+', 5A1, 8 )
    RETURN
    END
    SUBROUTINE FRAME1
    WRITE(9,110)
110  FORMAT ( ' P[250,5]T(S2)"OBOGS SIMULATION"' )
    WRITE(9,112)
112  FORMAT ( ' P[30,30]T(S1)"TIME =          SEC. "' )
    WRITE(9,114)

```

```

114 FORMAT ( ' P[280,95]T"1"P[280,245]T"0" ' )
    WRITE(9,118)
118 FORMAT ( ' P[280,295]T"1"P[280,445]T"0" ' )
    WRITE(9,120)
120 FORMAT ( ' P[400,80]T"BED #1" ' )
    WRITE(9,130)
130 FORMAT ( ' P[400,280]T"BED #2" ' )
    WRITE(9,140)
140 FORMAT ( ' P[20,255]T"INLET" ' )
    WRITE(9,150)
150 FORMAT ( ' P[5,275]T"PRESSURE" ' )
    WRITE(9,160)
160 FORMAT ( ' P[195,112]T"R.V." ' )
    WRITE(9,170)
170 FORMAT ( ' P[95,430]T"EXHAUST" ' )
    WRITE(9,180)
180 FORMAT ( ' P[115,450]T"GAS" ' )
    WRITE(9,190)
190 FORMAT ( ' P[624,268]T"P.O." ' )
    WRITE(9,192)
192 FORMAT ( ' P[680,112]T"B.P." ' )
    WRITE(9,193)
193 FORMAT ( ' P[720,412]V00000P[730,403]T"0%" ' )
    WRITE(9,195)
195 FORMAT ( ' P[720,358]V00000P[730,349]T"20%" ' )
    WRITE(9,198)
198 FORMAT ( ' P[720,132]V00000P[730,123]T"100%" ' )
    WRITE(9,200)
200 FORMAT ( ' P[275,100]V[575,100]V[575,250]V[275,250]V[275,100] ' )
    WRITE(9,210)
210 FORMAT ( ' P[275,300]V[575,300]V[575,450]V[275,450]V[275,300] ' )
    WRITE(9,300)
300 FORMAT ( ' P[575,182]V[670,182]V[670,132]V[720,132]V[720,412] ' )
    WRITE(9,310)
310 FORMAT ( ' V[670,412]V[670,382]V[575,382]P[575,182] ' )
    WRITE(9,400)
400 FORMAT ( ' V[600,182]V[600,267]V[605,272]V[600,277]V[600,362] ' )
    WRITE(9,410)
410 FORMAT ( ' V[575,382]P[620,182]V[670,182]V[670,362]V[620,362] ' )
    WRITE(9,450)
450 FORMAT ( ' V[620,277]V[615,272]V[620,267]V[620,182] ' )
    WRITE(9,460)
460 FORMAT ( ' P[720,282]V[750,282]V[750,282]V[720,282] ' )
    WRITE(9,500)
500 FORMAT ( ' P[275,182]V[240,182]V[240,132]V[180,132] ' )
    WRITE(9,510)
510 FORMAT ( ' V[180,182]V[118,182]V[118,262] ' )
    WRITE(9,520)
520 FORMAT ( ' P[275,182]V[240,182]P[180,182]V[138,182]V[138,262]
1 ' )
    WRITE(9,540)
540 FORMAT ( ' P[118,282]V[118,420]V[138,420]V[138,382] ' )
    WRITE(9,600)
600 FORMAT ( ' V[180,382]V[180,412]V[240,412]V[240,382]V[275,382] ' )
    WRITE(9,610)
610 FORMAT ( ' P[180,262]V[80,262]V[80,282] ' )
    WRITE(9,700)
700 FORMAT ( ' V[180,282]V[180,362]V[138,362]V[138,282]P[275,362] ' )
    WRITE(9,710)
710 FORMAT ( ' P[275,362]V[240,362]V[240,182]P[180,182]V[180,262] ' )
    WRITE(9,730)
730 FORMAT ( ' P[630,182]V[630,187]V[640,182] ' )
    WRITE(9,735)

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735 FORMAT ( ' P[630,182]V[630,177]V[640,182] ' )
WRITE(9,740)
740 FORMAT ( ' P[630,362]V[630,367]V[640,362] ' )
WRITE(9,750)
750 FORMAT ( ' P[630,382]V[630,377]V[640,382] ' )
RETURN
END
SUBROUTINE NEWTIME ( TIME,NW )
WRITE(9,100) NW,TIME
100 FORMAT ( ' W(N'I1')P[110,30]T(S1)'F6.2' ' ' )
RETURN
END
SUBROUTINE FRAME2 ( NBED,NW )
IF ( NBED .EQ. 1 ) THEN
WRITE(9,710)NW
710 FORMAT ( ' W(N'I1')P[180,262]V[240,362] ' )
ELSE
WRITE(9,720)NW
720 FORMAT ( ' W(N'I1')P[180,262]V[240,162] ' )
END IF
WRITE(9,730)NW
730 FORMAT ( ' W(N'I1')P[630,162]V[630,167]V[640,162] ' )
WRITE(9,735)
735 FORMAT ( ' P[630,182]V[630,177]V[640,182] ' )
WRITE(9,740)NW
740 FORMAT ( ' W(N'I1')P[630,362]V[630,367]V[640,362] ' )
WRITE(9,750)
750 FORMAT ( ' P[630,382]V[630,377]V[640,382] ' )
IF ( NBED .EQ. 1 ) THEN
WRITE(9,800)NW
800 FORMAT ( ' W(N'I1')P[180,282]V[240,382] ' )
WRITE(9,805)
805 FORMAT ( ' P[240,162]V[180,162]P[240,182]V[180,182] ' )
WRITE(9,810)NW
810 FORMAT ( ' W(N'I1')P[113,272]V[143,272] ' )
WRITE(9,815)
815 FORMAT ( ' P[136,268]V[]V[143,272]V[136,278] ' )
WRITE(9,820)NW
820 FORMAT ( ' W(N'I1')P[590,372]V[625,372] ' )
WRITE(9,825)
825 FORMAT ( ' P[620,369]V[]V[625,372]V[620,375] ' )
WRITE(9,830)NW
830 FORMAT ( ' W(N'I1')P[610,320]V[610,290] ' )
WRITE(9,835)
835 FORMAT ( ' P[607,295]V[]V[610,290]V[613,295] ' )
WRITE(9,840)NW
840 FORMAT ( ' W(N'I1')P[610,172]V[585,172] ' )
WRITE(9,845)
845 FORMAT ( ' P[590,169]V[]V[585,172]V[590,175] ' )
WRITE(9,850)NW
850 FORMAT ( ' W(N'I1')P[128,352]V[128,392] ' )
WRITE(9,855)
855 FORMAT ( ' P[124,385]V[]V[128,392]V[132,385] ' )
WRITE(9,860)NW
860 FORMAT ( ' W(N'I1')P[638,172]C[632,166] ' )
WRITE(9,865)
865 FORMAT ( ' P[645,172]V11117777111177771111000 ' )
WRITE(9,870)NW
870 FORMAT ( ' W(N'I1')P[650,372]C[643,372] ' )
WRITE(9,880)
880 FORMAT ( ' P[667,372]V11117777111100 ' )
ELSE
WRITE(9,900)NW

```



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900 FORMAT ( ' W(N'I1')P[180,282]V[240,182]' )
WRITE(9,905)
905 FORMAT ( ' P[180,382]V[240,382]P[180,382]V[240,382]' )
WRITE(9,910)NW
910 FORMAT ( ' W(N'I1')P[113,272]V[143,272]' )
WRITE(9,915)
915 FORMAT ( ' P[138,288]V[]V[143,272]V[138,278]' )
WRITE(9,920)NW
920 FORMAT ( ' W(N'I1')P[590,172]V[615,172]' )
WRITE(9,925)
925 FORMAT ( ' P[608,188]V[]V[615,172]V[608,178]' )
WRITE(9,930)NW
930 FORMAT ( ' W(N'I1')P[610,222]V[610,252]' )
WRITE(9,935)
935 FORMAT ( ' P[608,245]V[]V[610,252]V[614,245]' )
WRITE(9,940)NW
940 FORMAT ( ' W(N'I1')P[610,372]V[580,372]' )
WRITE(9,945)
945 FORMAT ( ' P[587,368]V[]V[580,372]V[587,378]' )
WRITE(9,950)NW
950 FORMAT ( ' W(N'I1')P[159,372]V[128,372]V[128,390]' )
WRITE(9,955)
955 FORMAT ( ' P[124,381]V[]V[128,390]V[132,381]' )
WRITE(9,960)NW
960 FORMAT ( ' W(N'I1')P[650,172]C[643,172]' )
WRITE(9,965)
965 FORMAT ( ' P[657,172]V11117777111100' )
WRITE(9,970)NW
970 FORMAT ( ' W(N'I1')P[638,372]C[633,366]' )
WRITE(9,980)
980 FORMAT ( ' P[645,372]V11117777111177770000' )
END IF
RETURN
END
SUBROUTINE REGISOUT
C SETS VT125 BACK INTO TEXT MODE
LOGICAL ALPHA
DIMENSION ALPHA(2)
DATA ALPHA / 27, '\ ' /
TYPE 10, ALPHA
10 FORMAT ( '+', 5A1, $ )
RETURN
END
SUBROUTINE DELAY ( NTICKS )
TYPE 100,NTICKS
100 FORMAT ( '+S(T<'I3'>)', $ )
RETURN
END
SUBROUTINE SCALEM ( Y,IYABS,VV,RANGE )
DY = (( VV - Y ) * 300.0 ) / RANGE
IDY = IFIX ( DY )
IYABS = IDY + 90
RETURN
END
SUBROUTINE STIME ( TIME,IXABS,RANGE,AXLEN,SHIFT )
INTEGER SHIFT
DX = ( TIME * AXLEN ) / RANGE
IDX = IFIX ( DX )
IXABS = IDX + SHIFT
RETURN
END
SUBROUTINE FRAME
COMMON/SYST/DT,PSUP,POUT,TF,WBRL,VS,V0,IIN,TCYC

```

```

COMMON/NPRINT/NOU1
DIMENSION T(10)
DELT = TF/10.0
DO I=1,10
T(I)=I*DELT
END DO
TYPE 10
10 FORMAT ( ' !P[130,390]V[+80,]V[,+5]' , $ )
DO I=1,9
TYPE 12
12 FORMAT ( ' !P[, -5]V[+80,]V[,+5]' , $ )
END DO
TYPE 20
20 FORMAT ( ' !P[120,398]T"O.O"' , $ )
TYPE 21 , T(1),T(2)
21 FORMAT ( ' !P[160,398]T" 'F5.1' "P[220,398]T" 'F5.1' "' , $ )
TYPE 22 , T(3),T(4)
22 FORMAT ( ' !P[280,398]T" 'F5.1' "P[340,398]T" 'F5.1' "' , $ )
TYPE 23 , T(5),T(6)
23 FORMAT ( ' !P[400,398]T" 'F5.1' "P[460,398]T" 'F5.1' "' , $ )
TYPE 24 , T(7),T(8)
24 FORMAT ( ' !P[520,398]T" 'F5.1' "P[580,398]T" 'F5.1' "' , $ )
TYPE 25 , T(9),T(10)
25 FORMAT ( ' !P[640,398]T" 'F5.1' "P[700,398]T" 'F5.1' "' , $ )
TYPE 30
30 FORMAT ( ' !P[350,430]T"TIME (SEC.)"' , $ )
TYPE 40
40 FORMAT ( ' !P[130,390]V[, -30]V[-5,]' , $ )
DO I=1,9
TYPE 50
50 FORMAT ( ' !P[+5,]V[, -30]V[-5,]' , $ )
END DO
TYPE 51
51 FORMAT ( ' !P[70,180]T[+0,+16]"OUTPUT"' , $ )
TYPE 53 , PSUP
53 FORMAT ( ' !P[530,34]T[+9,+0]"PSUP = "T" 'F5.2' "T" PSIA"' , $ )
TYPE 54 , POUT
54 FORMAT ( ' !P[530,52]T"POUT = "T" 'F5.2' "T" PSIA"' , $ )
TYPE 55 , WBRL
55 FORMAT ( ' !P[530,70]T"WBRL = "T" 'F5.2' "T" STD LIT/MIN"' , $ )
IF(NOUT1.EQ.1)THEN
57 TYPE 60
60 FORMAT ( ' !P[290,5]T"* OXYGEN MOLE FRACTION *"' , $ )
TYPE 62
62 FORMAT ( ' !P[95,383]T"O.O"P[95,353]T"O.1"P[95,323]T"O.2"' , $ )
TYPE 64
64 FORMAT ( ' !P[95,293]T"O.3"P[95,263]T"O.4"P[95,233]T"O.5"' , $ )
TYPE 66
66 FORMAT ( ' !P[95,203]T"O.6"P[95,173]T"O.7"P[95,143]T"O.8"' , $ )
TYPE 68
68 FORMAT ( ' !P[95,113]T"O.9"P[95,83]T"1.0"' , $ )
ELSE IF(NOUT1.EQ.2) THEN
TYPE 80
80 FORMAT ( ' !P[290,5]T"* INLET MASS FLOWRATE (KG/SEC) *"' , $ )
TYPE 82
82 FORMAT ( ' !P[85,383]T"- .02"P[85,353]T"- .01"P[95,323]T"O.O"' , $ )
TYPE 84
84 FORMAT ( ' !P[95,293]T".01"P[95,263]T".02"P[95,233]T".03"' , $ )
TYPE 86
86 FORMAT ( ' !P[95,203]T".04"P[95,173]T".05"P[95,143]T".06"' , $ )
TYPE 88
88 FORMAT ( ' !P[95,113]T".07"P[95,83]T".08"' , $ )
ELSE IF(NOUT1.EQ.3) THEN

```

1

```
90      TYPE 90
      FORMAT ( ' !P[290,5]T" * OUTLET MASS FLOWRATE (KG/SEC) - " ', $)
      TYPE 82
      TYPE 84
      TYPE 86
      TYPE 88
      ELSE
      GO TO 57
      END IF
      RETURN
      END
```

APPENDIX C.

These are the corrected equations for the van der Vlist paper (8). These are for the binary mixture at total pressure (constant) P. The six unknowns (A's and B's) are found in terms of known quantities (G's and W's). See the paper for the complete details.

Essentially, six equations in six unknowns are solved. The equations are:

$$G_0 = P * A_1 \quad (1)$$

$$G_1 = 2 * P * A_2 - A_1 + B_1 + 2 * P * B_2 + 3 * P^2 * B_3 \quad (2)$$

$$G_2 = 3 * P * A_3 - 2 * A_2 - 2 * B_2 - 3 * 2 * P * B_3 \quad (3)$$

$$G_3 = - 3 * A_3 + 3 * B_3 \quad (4)$$

$$W_1 = P * A_1 + P^2 * A_2 + P^3 * A_3 \quad (5)$$

$$W_2 = P * B_1 + P^2 * B_2 + P^3 * B_3 \quad (6)$$

These equations give the following solution:

$$A_1 = \frac{G_0}{P}$$

$$A_2 = \frac{- 6 * W_2 - 3 * W_1 + 2 * G_3 * P^3 + 3 * G_2 * P^2 + 6 * G_1 * P + 9 * G_0}{3 * P^2}$$

$$A_3 = - \frac{- 6 * W_2 - 6 * W_1 + 2 * G_3 * P^3 + 3 * G_2 * P^2 + 6 * G_1 * P + 12 * G_0}{3 * P^3}$$

$$B_1 = \frac{G_3 * P^3 + G_2 * P^2 + G_1 * P + G_0}{P}$$

$$B_2 = - \frac{3 * W_2 + 6 * W_1 + 2 * G_3 * P^3 - 3 * G_1 * P - 9 * G_0}{3 * P^2}$$

$$B_3 = - \frac{-6 * W_2 - 6 * W_1 + G_3 * P^3 + 3 * G_2 * P^2 + 6 * G_1 * P + 12 * G_0}{3 * P^3}$$

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